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Page 1

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L4 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:610730 CAPLUS

DOCUMENT NUMBER: 139:161501

TITLE: Purification and characterization of elisabethatriene cyclase from *Pseudopterogorgia elisabethae* and use for production of elisabethatriene

INVENTOR(S): Kerr, Russell; Kohl, Amber; Lopez, Jose

PATENT ASSIGNEE(S): Florida Atlantic University, USA

SOURCE: PCT Int. Appl., 22 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003065001	A2	20030807	WO 2003-US2299	20030127
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

US 2003153052 A1 20030814 US 2003-351766 20030127

PRIORITY APPL. INFO.: US 2002-351984 P 20020125

AB An enzyme having diterpene cyclase activity has been purified from *Pseudopterogorgia elisabethae* using a series of chromatog. steps. The purified enzyme has an apparent mol. wt. of about 47 kilodaltons and an isoelec. point of about 5.1. The purified enzyme catalyzed the cyclization of geranyl geranyl diphosphate to elisabethatriene. The invention provides a method for cyclizing geranyl geranyl diphosphate for prodn. of elisabethatriene. The elisabethatriene thus formed can be used as a substrate to produce other mols. involved in pseudopterogorgia synthesis, such as elisabethadiol, pseudopterogorgia aglycon, and pseudopterogorgia A.

IT 433717-71-69, Elisabethadione

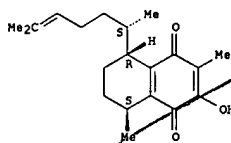
RL: PNU (Preparation, unclassified); PREP (Preparation) (purifn. and characterization of elisabethatriene cyclase from *Pseudopterogorgia elisabethae* and use for prodn. of elisabethatriene)

RN 433717-71-6 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)



L4 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:406303 CAPLUS

DOCUMENT NUMBER: 139:146643

TITLE: Identification of anti-inflammatory diterpenes from the marine gorgonian *Pseudopterogorgia elisabethae* Ata, Athar; Kerr, Russell G.; Moya, Claudia E.; Jacobs, Robert S.

CORPORATE SOURCE: Center for Molecular Biology and Biotechnology, Department of Chemistry and Biochemistry, Florida Atlantic University, Boca Raton, FL 33431, USA

SOURCE: Tetrahedron (2003), 59(23), 4215-4222

CODEN: TETRAH; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

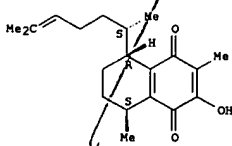
LANGUAGE: English

AB Anal. of the terpene metabolites of *Pseudopterogorgia elisabethae* collected from the Florida Keys has resulted in the identification of a novel hydroquinone, elisabethadione (5), as well as new pseudopterogorgia and seco-pseudopterogorgia. Anti-inflammatory assays indicate that elisabethadione is more potent than the well characterized pseudopterogorgia A and E. This report also describes the co-occurrence of pseudopterogorgia and seco-pseudopterogorgia, diterpenes with amphilectane and serrulatane skeletons, resp. This together with our previously described isolation of elisabethatriene as the sole diterpene cyclase product in *P. elisabethae* suggests that the amphilectane and serrulatane families of diterpenes are derived from the same geranylgeranyl diphosphate cyclase product.

IT RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (anti-inflammatory diterpenes from marine gorgonian *Pseudopterogorgia elisabethae*)

RN 433717-71-6 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:280878 CAPLUS

DOCUMENT NUMBER: 139:85507

TITLE: Unified strategy for the synthesis of (-)-elisapterosin B and (-)-colombiasin A Kim, Angie I.; Rychnovsky, Scott D.

CORPORATE SOURCE: Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA

SOURCE: Angewandte Chemie, International Edition (2003), 42(11), 1267-1270

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH &amp; Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (-)-Elisapterosin B was synthesized using an intramol. [5 + 2] cycloaddn. as a key step. (-)-Colombiasin A was also synthesized via the same route, but with an intramol. thermal [4 + 2] Diels-Alder reaction as the final step.

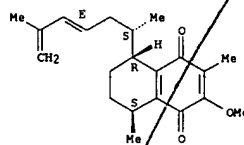
IT 552824-51-8P 552824-55-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of (-)-elisapterosin B and (-)-colombiasin A from a chiral aldehyde via either an intramol. [5+2] cycloaddn. or Diels-Alder reaction)

RN 552824-51-8 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

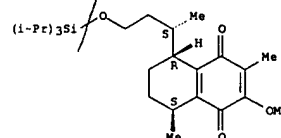
Absolute stereochemistry.

Double bond geometry as shown.



RN 552824-55-2 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S)-1-methyl-3-[[tris(1-methylethyl)silyl]oxy]propyl]-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:52625 CAPLUS  
DOCUMENT NUMBER: 137:98953  
TITLE: Anti-inflammatory compounds derived from Pseudopterogorgia elisabethae  
INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

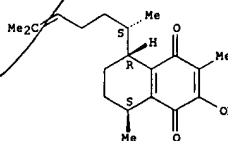
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-994666	20011127
			US 2000-235460P	P 20000922

PRIORITY APPLN. INFO.: MARPAT 137:98953

OTHER SOURCE(S):  
AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprise the administration of a pseudopteroin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopteroin and compds. related to pseudopteroin are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 604 aq. MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopteroin, seco-pseudopteroin, and elisabethadiol. Pseudopteroin had high anti-inflammatory activity.

IT 433717-71-6, Elisabethadione  
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses) (anti-inflammatory compds. from Pseudopterogorgia elisabethae)  
RN 433717-71-6 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:428919 CAPLUS  
DOCUMENT NUMBER: 137:15779  
TITLE: Anti-inflammatory compounds derived from Pseudopterogorgia elisabethae  
INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
PATENT ASSIGNEE(S): The Regents of the University of California, USA  
SOURCE: PCT Int. Appl., 44 pp.  
CODEN: PIXX02  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GR, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM  
RV: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002041521 A5 20020611 AU 2002-41521 20011127  
EP 1339729 A2 20030903 EP 2001-988191 20011127  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.: US 2000-253160P P 20001128  
WO 2001-US44334 W 20011127

OTHER SOURCE(S): MARPAT 137:15779

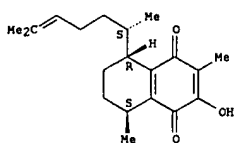
AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopteroin and compds. related to pseudopteroin are disclosed. Examples are provided demonstrating the anti-inflammatory, antiproliferative and analgesic activity of several compds. (pseudopteroin M, seco-pseudopteroin E, elisabethdione, etc.) isolated from P. elisabethae.

IT 433717-71-6P, Elisabethadione  
RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(pharmacol. activity of compds. derived from Pseudopterogorgia elisabethae)  
RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

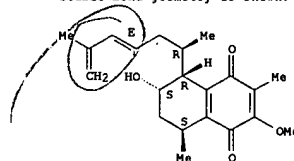
L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:11433 CAPLUS  
 DOCUMENT NUMBER: 136:279574  
 TITLE: Total synthesis of colombiasin A and determination of its absolute configuration  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Chemistry--A European Journal (2001), 7(24), 5359-5371  
 CODEN: CEUJED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The total synthesis of the recently reported marine natural product colombiasin A (I) and detn. of its abs. configuration are reported. Two Diels - Alder cycloaddns. and a palladium-catalyzed rearrangement are employed as key reactions to construct the tetracyclic framework of the target mol. The enantioselective synthesis of colombiasin A utilizes Mikami's [(S)-BINOL-TiCl2] catalyst to asym. introduce the first chiral center during the initial Diels - Alder reaction and, in conjunction with X-ray crystallog. anal. of a bromine contg. deriv., led to the assignment of the abs. configuration of the natural product.  
 IT 362650-95-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A and detn. of its abs. configuration)  
 RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



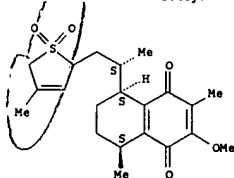
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:831849 CAPLUS  
 DOCUMENT NUMBER: 136:151319  
 TITLE: Towards colombiasin A  
 AUTHOR(S): Harrowven, David C.; Tye, Melloney J.  
 CORPORATE SOURCE: Department of Chemistry, The University of Southampton, Southampton, SO17 1BJ, UK  
 SOURCE: Tetrahedron Letters (2001), 42(49), 8709-8711  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A synthetic route to an diastereomerically unnatural analog I of colombiasin A (II) is described. Key features are an arene alkylation with a .gamma.-methylene-.gamma.-butyrolactone and an intramol. Diels-Alder cycloaddn.  
 IT 394739-50-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthetic studies directed towards colombiasin A)  
 RN 394739-50-5 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, (5R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

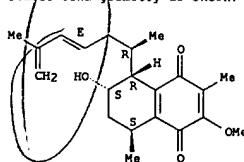


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:516801 CAPLUS  
 DOCUMENT NUMBER: 135:273093  
 TITLE: Total synthesis of Colombiasin A  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Angewandte Chemie, International Edition (2001), 40(13), 2482-2486  
 CODEN: ACHIEF; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:273093  
 AB The authors report the total synthesis of racemic colombiasin A (I) by a strategy which also delivered its C7 epimer as well as several other analogs.  
 IT 362650-95-1P 362651-05-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A)  
 RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

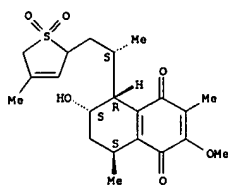
Relative stereochemistry.  
 Double bond geometry as shown.



RN 362651-05-6 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5S,6R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:895538 CAPLUS  
 DOCUMENT NUMBER: 134:160401  
 TITLE: Structurally diverse terpenoids from the sea whip *Pseudopterogorgia elisabethae* (Bayer)  
 AUTHOR(S): Rodriguez, A. D.; Shi, Y.-P.  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.  
 SOURCE: Tetrahedron (2000), 56(46), 9015-9023  
 CODEN: TETRA; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

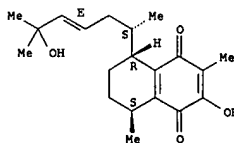
AB The extn. of a specimen of *Pseudopterogorgia elisabethae* from Colombia afforded three new diterpenes (I-III), a norditerpene (IV), and a tetrasternoditerpene (V). Metabolites IV and V contain unusual carbon skeletons that are previously undescribed and therefore constitute new classes of C19 and C16 rearranged terpenes, resp. Full details of the isolation and structure elucidation of I-V, which were established by spectroscopic methods including comprehensive 2D NMR measurements, are provided herein.

IT RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (terpenoids from sea whip *Pseudopterogorgia elisabethae*)

RN 325691-48-3 CAPLUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-[(1R,3E)-5-hydroxy-1,5-dimethyl-3-hexenyl]-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.  
 Double bond geometry as shown.  
 Currently available stereo shown.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:108327 CAPLUS  
 DOCUMENT NUMBER: 128:192798  
 TITLE: Formation of mansonones from naturally occurring para-benzoquinones  
 AUTHOR(S): Garcia, Esther; Mendoza, Virgilio; Agustin Guzman, J.  
 CORPORATE SOURCE: Instituto Investigaciones Químico-Biológicas, Universidad Michoacana San Nicolás de Hidalgo, Morelia, 58030, Mex.  
 SOURCE: Natural Product Letters (1997), 11(1), 67-72  
 CODEN: NPLEFF; ISSN: 1057-5634  
 PUBLISHER: Harwood Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

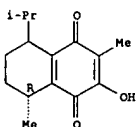
AB Cyclization of perezene and hydroxyperezene with HI, followed by Jones oxidn., converted them into isomansonone A and mansonone A, B, and C.

IT 203174-32-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of mansonones from perezene)

RN 203174-32-7 CAPLUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

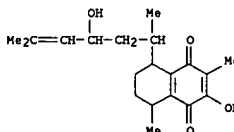
ACCESSION NUMBER: 1989:21335 CAPLUS  
 DOCUMENT NUMBER: 110:21335  
 TITLE: New marine diterpenoids, including a unique hydroperoxide, from a Caribbean gorgonian coral of the genus *Pseudopterogorgia*  
 AUTHOR(S): Harvis, Carl A.; Burch, Mark T.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Scripps Inst. Oceanogr., La Jolla, CA, 92093-0228, USA  
 SOURCE: Tetrahedron Letters (1988), 29(35), 4361-4  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Journal  
 DOCUMENT TYPE: English  
 OTHER SOURCE(S): CASREACT 110:21335

AB 4 New diterpenoids (I-IV) related to the aglycon components of the recently described pseudopterocins and seco-pseudopterocins have been isolated from an undescribed *Pseudopterogorgia* species from the Caribbean Sea. The new compds., described on the basis of their NMR properties and chem. interconversions, appear to be related, illustrating some interesting rearrangements of a tertiary hydroperoxide in this series.

IT RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (of gorgonian coral)

RN 118169-36-1 CAPLUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-(3-hydroxy-1,5-dimethyl-4-hexenyl)-3,8-dimethyl- (9CI) (CA INDEX NAME)



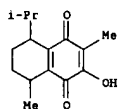
L4 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1967:105061 CAPLUS  
 DOCUMENT NUMBER: 66:105061  
 TITLE: Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Marini-Bettolo, Giovanni B.; Casinovi, Carlo G.; Galeffi, Corrado; Delle Monache, Franco; Del Guercio, G.  
 CORPORATE SOURCE: Univ. Cattolica, Rome, Italy  
 SOURCE: Annali dell'Istituto Superiore di Sanita (1966), 2(2-3), 327-41  
 CODEN: AIISSAW; ISSN: 0021-2571  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Italian

AB CA 64, 12728d. The wood of *M. altissima*, which is widely used for furniture making, was studied for the irritating and cardiokinetic substances it contains. By means of column chromatog., the crude CHCl<sub>3</sub> ext. of *M. altissima* was fractionated into 6 new quinones: red mansonone A (I), m. 117-18.degree., [ $\alpha$ ]<sub>D</sub> 200 680.degree. (c 0.2, CHCl<sub>3</sub>); gold-yellow mansonone B (II), 68-9.degree.; orange mansonone C (III), m. 134-8.degree.; orange mansonone D (IV), m. 173-5.degree.; orange-yellow mansonone E (V), m. 148-9.degree.; violet-mansonone F (VI), m. 214-15.degree.. Their structures were partially elucidated by chem. and spectroscopic analysis. A C15 skeleton which is a common feature for the compds. suggests a terpene origin. Two have the structure of oxaphenylene found the 1st time in biflorin. I was easily reduced in H<sub>2</sub>O with Na hydrosulfite. I was reduced with Zn in Ac<sub>2</sub>O and pyridine to yield the diacetate, m. 158-60.degree.. Ac<sub>2</sub>O and NaOAc yielded the acetate, b<sub>0</sub>.02 120.degree.. II, III, IV, and V were reduced by Na hydrosulfite and reoxidized by air. III with pyridine, Ac<sub>2</sub>O, and Zn yielded the diacetate, m. 156-8.degree.. Boiling with an acetic acid soln. of o-phenylenediamine yielded the quinoxaline, m. 103-4.degree.. IV did not react with Ac<sub>2</sub>O and NaOAc. With Zn and Ac<sub>2</sub>O and pyridine it gave a diacetyl deriv. With o-phenylenediamine and acetate V gave a deriv., m. 148-50.degree.. With Zn, Ac<sub>2</sub>O, and pyridine V gave a diacetate, m. 110.degree.. VI is very sensitive to light and changes with time, especially in soln.

IT 14375-53-2  
 RL: PRP (Properties)  
 (structure of)

RN 14375-53-2 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



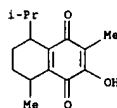
L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1966:67994 CAPLUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:12728d-h,12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Bettolo, G. B.; Marini; Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: Ist. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TETLEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sep'd. the CHCl<sub>3</sub> irritative fraction into 6 C15-quinones designated as mansonones A, B, C, D, E, and F. m. 117-18.degree. (C<sub>6</sub>H<sub>12</sub>), 68-9.degree. (C<sub>6</sub>H<sub>14</sub>), 134-8.degree. (C<sub>6</sub>H<sub>14</sub>), 173-5.degree. (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>6</sub>), 148-9.degree. (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree. (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C15H<sub>20</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -CMe:CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C19H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b<sub>0</sub>.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, alc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formulas is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Sandermann and Dietrichs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

IT 14375-53-2, Mansonone B  
 (structure of)

RN 14375-53-2 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

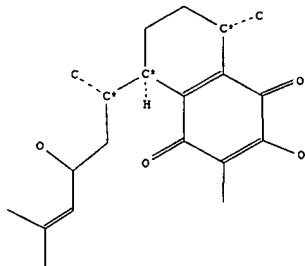
09/993,666

Page 7

=> d all 1-2

## L5 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 5095107  
 Beilstein Pref. RN (BPR): 118169-36-1  
 CAS Reg. No. (RN): 118169-36-1  
 Chemical Name (CN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Autonom Name (AUN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molac. Formula (MF): C20 H28 O4  
 Molecular Weight (MW): 332.44  
 Lawson Number (LN): 9791  
 File Segment (FS): relative configuration, Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 4527263  
 Tautomer ID (TAUTID): 4874682  
 Beilstein Citation (BSO): 6-08  
 Entry Date (DED): 1992/08/28  
 Update Date (DUPD): 1993/03/20



Fragment Notes:  
 Alternatively represents mirror image  
 Stereo Descriptor: rel

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1

L5 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN  
(Continued)

## UV and Visible Spectrum:

Description	Solvent	Absorption	Ext./Abs. Coeff.	Ref.
(.KW)	(.SOL)	(.AM)	(.EAC)	
		(nm)	(1/MOL*CM)	
Absorption maxima	methanol	326, 281, 223	4600, 7500, 15700	11
Absorption maxima	methanol	321, 279, 220	3100, 8900, 13200	11

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

L5 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN  
(Continued)

Autonom Name	1
MF	Molecular Formula
FW	Formular Weight
LN	Lawson Number
FS	File Segment
CTYPE	Compound Type
CONSID	Constitution ID
TAUTID	Tautomer ID
BSO	Beilstein Citation
ED	Entry Date
UPD	Update Date
INP	Isolation from Natural Product
IR	Infrared Spectrum
NMR	Nuclear Magnetic Resonance
UVS	UV and Visible Spectrum

## Isolation from Natural Product:

INP (INP): Pseudopterogorgia  
 Reference(s):  
 1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Nuclear Magnetic Resonance:

NMR Description (.KW): Chemical shifts  
 Nucleus (.NUC): <sup>1</sup>H  
 Solvents (.SOL): CDCl3  
 Reference(s):  
 1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## NMR

Description (.KW): Chemical shifts  
 Nucleus (.NUC): <sup>13</sup>C  
 Solvents (.SOL): benzene-d6  
 Reference(s):  
 1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Infrared Spectrum:

Descript	Solvent	Ref.	Note
ion			
(.KW)	(.SOL)		
Bands	CHCl3	11	1

## Reference(s):

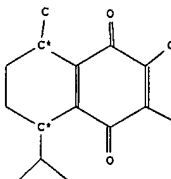
1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Notes(s):

1. 3000 - 1640 cm<sup>-1</sup> (-1)

## L5 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 2053092  
 Beilstein Pref. RN (BPR): 14375-53-2  
 CAS Reg. No. (RN): 14375-53-2  
 Chemical Name (CN): Mansonon B  
 Autonom Name (AUN): 2-hydroxy-5-isopropyl-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molac. Formula (MF): C15 H20 O3  
 Molecular Weight (MW): 248.32  
 Lawson Number (LN): 9296  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 1884852  
 Tautomer ID (TAUTID): 2003770  
 Beilstein Citation (BSO): 5-08  
 Entry Date (DED): 1989/06/29  
 Update Date (DUPD): 1992/06/02



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonom Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
INP	Isolation from Natural Product	2
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1
RSTR	Related Structure	1
UVS	UV and Visible Spectrum	1

## Related Structure:



L5 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN  
(Continued)

RSTR

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

Isolation from Natural Product:

INP

(INP): M. altissima

Reference(s):

1. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAW, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

INP

(INP): a. Mansonia Altissima Cher.

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

Melting Point:

Value |Ref.

(MP) |

(Cel) |

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68 - 69 |1, 2

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857
2. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAW, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

UV and Visible Spectrum:

Description |Ref.

(.KW) |

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Absorption maxima |1

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

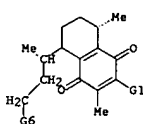
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L7 ANSWER 1 OF 3 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 137:98953 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.:			US 2000-235160P	20000922

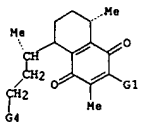
AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprise the administration of a pseudopterostin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an Cl-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 60% aq. MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterostins, seco-pseudopterostins, and elisabethadiol. Pseudopterostins had high anti-inflammatory activity.

## MSTR 3



G1 = OH  
 MPL: claim 21  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L7 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G1 = OH  
 MPL: claim 21  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L7 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 137:15779 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): The Regents of the University California, USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 AU 2002041521 A5 20020611 AU 2002-41521 20011127  
 EP 1339729 A2 20030903 EP 2001-988191 20011127  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AB, FK  
 PRIORITY APPLN. INFO.:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000-253160P			20001128	
WO 2001-US44334			20011127	

AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. Examples are provided demonstrating the anti-inflammatory, antiproliferative and analgesic activity of several compds. (pseudopterostin M, seco-pseudopterostin E, elisabethdione, etc.) isolated from P. elisabethae.

## MSTR 3

L7 ANSWER 3 OF 3 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 110:4187 MARPAT  
 TITLE: Composition and method for rapid differentiation of  
 viable fungi from bacteria using polyene antibiotics  
 INVENTOR(S): Cichanowicz, Peggy Woodruff; Belly, Robert Troconis  
 PATENT ASSIGNEE(S): Eastman Kodak Co., USA  
 SOURCE: Eur. Pat. Appl., 22 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 261931	A2	19880330	EP 1987-308380	19870922
EP 261931	A3	19891011		

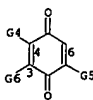
R: CH, DE, FR, GB, LI  
 CA 1290226 A1 19911008 CA 1986-523203 19861118  
 US 1986-910923 19860924  
 PRIORITY APPLN. INFO.:

AB Viable fungi are rapidly differentiated from viable bacteria by incubation with a compn. contg. a polyene antibiotic which affects membrane function in fungi and a compd. [e.g. a RIND compd. (reducible compd. which undergoes intramol. nucleophilic displacement) such as quinone I, where R1 = (R5)mN(R6)QX; R2, R4 = H, (substituted) alkyl or aryl, electron-withdrawing group; R3 = R1, R2; or R3R4 complete a (substituted) strained fused carbocyclic ring; R5 = (substituted) Cl-2 alkylene; R6 = (substituted) alkyl, cycloalkyl, aryl, or heterocycle; Q = C(O), C(S); X = shiftable detectable species which provides a detectable species when released; m = 0, 1] which is normally reducible by both fungi and bacteria. The antibiotic selectively inhibits the redn. of the reducible compd. by the fungi but does not affect the reducing capacity of the bacteria. A soln. contg. RIND compd. II, glucose, trimethyl-1,4-benzoquinone (electron transfer agent), buffer, and filipin (polyene antibiotic) at various dilns. was incubated with suspensions of various bacteria and fungi at 37 degrees. for 30 min, and the difference in relative fluorescence before and after incubation was measured with excitation at 540 nm and emission at 620 nm. The percent inhibition of redn. of II at 0.52 mg filipin/mL was: Escherichia coli, 0; Staphylococcus aureus, 8.6; Candida albicans, 71.0; Aspergillus flavus, 42.5.

## MSTR 1B

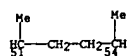
G2—G1

G1 = 6



G5 = OMe  
 G7 = alkylene<(1-2)> (SO (1-) G11)  
 G4 + G6 = 51-4 54-3

L7 ANSWER 3 OF 3 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



MPL: claim 4

=> d his

(FILE 'HOME' ENTERED AT 15:12:18 ON 30 OCT 2003)

FILE 'REGISTRY' ENTERED AT 15:12:24 ON 30 OCT 2003

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 11 S L1 FULL

FILE 'CAPLUS' ENTERED AT 15:13:52 ON 30 OCT 2003

L4 13 S L3

FILE 'BEILSTEIN' ENTERED AT 15:18:24 ON 30 OCT 2003

L5 2 S L3

FILE 'MARPAT' ENTERED AT 15:22:21 ON 30 OCT 2003

L6 0 S L3

L7 3 S L3 FULL

L19 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:48793 CAPLUS

DOCUMENT NUMBER: 112:48793

TITLE: Pseudopterins and their synthetic derivatives as anticancer, antiinflammatory and analgesic drugs

INVENTOR(S): Jacobs, Robert S.; Fenical, William H.

PATENT ASSIGNEE(S): University of California, USA

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8901334	A1	19890223	WO 1988-US2695	19880808
W: JP				
RM: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4849410	A	19890718	US 1987-85628	19870814
CA 1317591	A1	19930511	CA 1988-574076	19880808
PRIORITY APPLN. INFO.:			US 1987-85628	19870814
			US 1985-723214	19850415

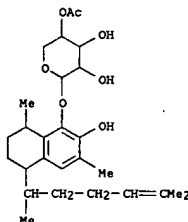
OTHER SOURCE(S): MARPAT 112:48793

AB The title compds. I (R1-R4 = H, Cl-6 acyl; R5 = H, Me, CH<sub>2</sub>OH; R6 = Cl-10 hydrocarbyl) are antiinflammatory, anticancer and analgesic drugs. I (R1-R5 = H, R6 = 2-methyl-1-propenyl) (II) administered i.p. at 1-5 mg/kg, almost doubled the survival time of mice with P388 leukemia. II was extd. from Pseudopterogorgia with 10% MeOH in CHCl<sub>3</sub>, followed by solvent evapn., reextr. with CHCl<sub>3</sub> and purifn. by silica gel chromatog.

IT 106665-01-4 106665-02-5 106665-03-6  
 RL: BIOL (Biological study)  
 (anticancer and antiinflammatory and analgesic drug)

RN 106665-01-4 CAPLUS

CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



L19 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1987:63306 CAPLUS

DOCUMENT NUMBER: 107:233406

TITLE: The seco-pseudopterins, new anti-inflammatory diterpene-glycosides from a Caribbean gorgonian octocoral of the genus Pseudopterogorgia

AUTHOR(S): Look, Sally A.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Univ. California, San Diego, La Jolla, CA, 92093, USA

SOURCE: Tetrahedron (1987), 43(15), 3363-70

CODEN: TETRA8; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

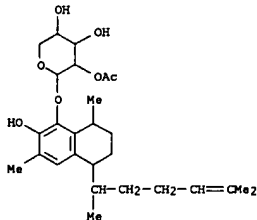
AB A new class of diterpene-pentosides, the seco-pseudopterins A-D (I, II, III, and IV) were isolated from a Caribbean sea whip of the genus Pseudopterogorgia. The new compds. are arabinose glycosides possessing aglycone of the serrulata class, the compds. in the series are monoacetate positional isomers, and they are related to the recently described pseudopterins by bond cleavage at the C5 - C13 positions. The seco-pseudopterins possess potent anti-inflammatory and analgesic activities equiv. to com. anti-inflammatory drugs. The structures of these new compds. are suggested on the basis of comprehensive spectral analyses and chem. transformations.

IT 111397-51-4 111466-65-0 111466-66-1

RL: BIOL (Biological study)  
 (of gorgonian octocoral, isolation and mol. structure and anti-inflammatory activity of)

RN 111397-51-4 CAPLUS

CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 2-acetate (9CI) (CA INDEX NAME)



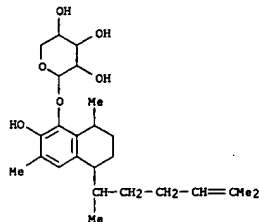
RN 111466-65-0 CAPLUS

CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)

L19 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

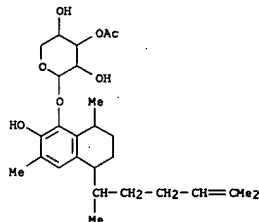
RN 106665-02-5 CAPLUS

CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

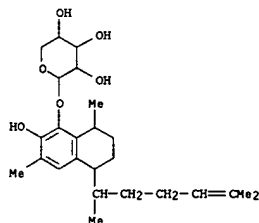


RN 106665-03-6 CAPLUS

CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

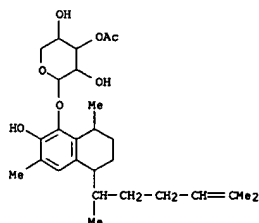


L19 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 111466-66-1 CAPLUS

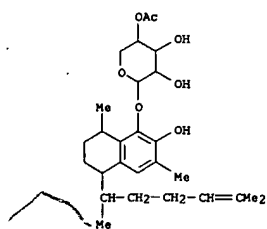
CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate (9CI) (CA INDEX NAME)



RN 111466-67-2 CAPLUS

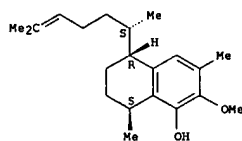
CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate (9CI) (CA INDEX NAME)

L19 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT 111397-54-7P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and NMR of)  
 RN 111397-54-7 CAPLUS  
 CN 1-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

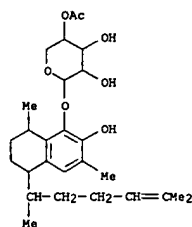


L19 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1987:84986 CAPLUS  
 DOCUMENT NUMBER: 106:84986  
 TITLE: Pseudopterosin and its synthetic derivatives  
 INVENTOR(S): Jacobs, Robert S.; Fenical, William H.  
 PATENT ASSIGNEE(S): University of California, Berkeley, USA  
 SOURCE: Eur. Pat. Appl., 31 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

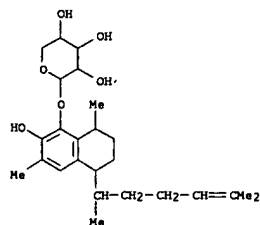
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 198689	A2	19861022	EP 1986-302711	19860411
EP 198689	A3	19870610		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4745104	A	19880517	US 1985-723214	19850415
CA 1288771	A1	19910910	CA 1986-505110	19860326
ZA 8602488	A	19861126	ZA 1986-2488	19860403
DK 8601626	A	19861016	DK 1986-1626	19860410
AU 8656065	A1	19861023	AU 1986-56065	19860414
ES 553952	A1	19871101	ES 1986-553952	19860414
JP 62036395	A2	19870217	JP 1986-85238	19860415
JP 2748001	B2	19980506		

PRIORITY APPLN. INFO.: US 1985-723214 19850415  
 AB The title compds. I [R1-R4 = H, Cl-6 acyl; R5 = H, HOCH2; R6 = (unsubstituted hydrocarbonyl) were isolated from Caribbean gorgonians or prepd. and tested for analgesic and antiinflammatory activity. Thus, pseudopterosin A (R1-R5 = H, R6 = Me2C:CH) was acetylated with Ac2O in pyridine to give 791 I (R1-R4 = Ac, R5 = H, R6 = Me2C:CH) (II). In the phenylquinone writhing test in mice 25 mg II/kg s.c. reduced writhing 34%.  
 IT 106665-01-4 106665-02-5 106665-03-6  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 RN 106665-01-4 CAPLUS  
 CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

L19 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

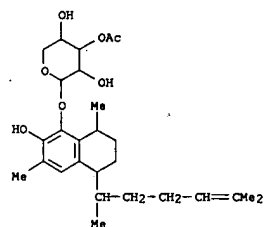


RN 106665-02-5 CAPLUS  
 CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



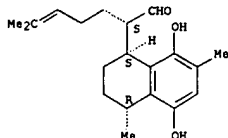
RN 106665-03-6 CAPLUS  
 CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

L19 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



L19 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1985:611133 CAPLUS  
 DOCUMENT NUMBER: 103:211133  
 TITLE: Eremophilane and serrulane terpenoids from  
*Eremophila rotundifolia*  
 AUTHOR(S): Abell, Andrew D.; Massy-Westropp, Ralph A.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. Adelaide, Adelaide, 5001,  
 Australia  
 SOURCE: Australian Journal of Chemistry (1985), 38(8), 1263-9  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The new terpenoids 9-oxoeremophila-10,11(13)-dien-12-al (I) and  
 5,8-dihydroxyserrulat-14-en-18-al (II) were isolated from *E. rotundifolia*.  
 Their abs. stereochem. was established by chem. correlation with known  
 compds.  
 IT 99305-32-5  
 RL: BIOL (Biological study)  
 (from *Eremophila rotundifolia*, structure of)  
 RN 99305-32-5 CAPLUS  
 CN 1-Naphthaleneacetaldehyde, 1,2,3,4-tetrahydro-5,8-dihydroxy-4,7-dimethyl-  
 .alpha.-(4-methyl-3-pentenyl)-, [1S-[1.alpha.(R\*),4.beta.]]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

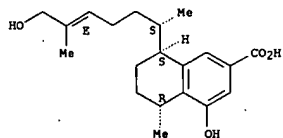


IT 99305-21-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT.  
 (Reactant or reagent)  
 (prepn. and reaction of)  
 RN 99305-21-2 CAPLUS  
 CN 1,4-Naphthalenediol, 5,6,7,8-tetrahydro-8-[1-(hydroxymethyl)-5-methyl-4-  
 hexenyl]-2,5-dimethyl-, [5R-[5.alpha.,8.beta.(S\*)]]- (9CI) (CA INDEX  
 NAME)

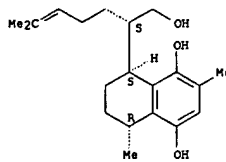
Absolute stereochemistry.

L19 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1980:146967 CAPLUS  
 DOCUMENT NUMBER: 92:146967  
 TITLE: The chemistry of *Eremophila* spp. XI. The absolute  
 configuration of dihydroxyserrulatic acid  
 Croft, Kevin D.; Ghisalberti, Emilio L.; Jefferies,  
 Phillip R.; Stuart, Alan D.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands,  
 6009, Australia  
 SOURCE: Australian Journal of Chemistry (1979), 32(9), 2079-83  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The (1'S)-configuration of dihydroxyserrulatic acid (I), isolated from *E.*  
*serrulata*, was detd. by transformation into the (1'S)-  
 dimethylhexylnaphthalene II and by synthesis of its enantiomer III from  
 (R)-citronellal.  
 IT 65003-68-1  
 RL: PRP (Properties)  
 (abs. configuration of)  
 RN 65003-68-1 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-  
 1,5-dimethyl-4-hexenyl)-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

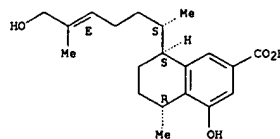


L19 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



L19 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1978:7095 CAPLUS  
 DOCUMENT NUMBER: 88:7095  
 TITLE: The chemistry of *Eremophila* spp.-VI. Stereochemistry  
 and crystal structure of dihydroxyserrulatic acid  
 Croft, Kevin D.; Ghisalberti, Emilio L.; Jefferies,  
 Philip R.; Raston, Colin L.; White, Allan H.; Hall,  
 Sydney R.  
 CORPORATE SOURCE: Crystallogr. Cent., Univ. West. Australia, Nedlands,  
 Australia  
 SOURCE: Tetrahedron (1977), 33(12), 1475-80  
 CODEN: TETRA8; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The structure of the title compd. (I) (from *E. serrulata*), a diterpenoid  
 analog of codinene, was detd. I was characterized by chem. and spectral  
 data and its relative stereochem. established by x-ray diffraction at 295  
 K. 5td. degrdn. of I gave the naphthalene II.  
 IT 65003-68-1P  
 RL: PREP (Preparation)  
 (from *Eremophila serrulata*, structure detn. of)  
 RN 65003-68-1 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-  
 1,5-dimethyl-4-hexenyl)-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

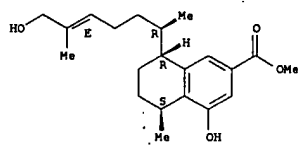


IT 65003-60-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and acetylation of)  
 RN 65003-60-3 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-  
 1,5-dimethyl-4-hexenyl)-5-methyl-, methyl ester,  
 [5.alpha.,8.beta.(1S\*,4E)]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.  
 Double bond geometry as shown.



L19 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



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(FILE 'HOME' ENTERED AT 12:06:10 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 12:06:15 ON 28 MAY 2003

L1               STRUCTURE UPLOADED  
L2               STRUCTURE UPLOADED  
L3               2 S L1 FULL  
L4               0 S L2 FULL

FILE 'CAPLUS' ENTERED AT 12:07:20 ON 28 MAY 2003

L5               1 S L3

FILE 'BEILSTEIN' ENTERED AT 12:07:52 ON 28 MAY 2003

L6               2 S L1 FULL  
L7               0 S L2 FULL

FILE 'MARPAT' ENTERED AT 12:09:51 ON 28 MAY 2003

L8               100 S L3 FULL

FILE 'REGISTRY' ENTERED AT 12:12:09 ON 28 MAY 2003

L9               STRUCTURE UPLOADED  
L10              106 S L9 FULL  
L11               2 S L1 FULL  
L12               1 S L9  
L13              106 S L9 FULL  
L14               79 S L13 AND 2/NR

FILE 'CAPLUS' ENTERED AT 12:16:45 ON 28 MAY 2003

L15              110 S L14  
L16               97 S L15 NOT PY>=2000

FILE 'REGISTRY' ENTERED AT 12:17:54 ON 28 MAY 2003

L17               STRUCTURE UPLOADED  
L18               34 S L17 FULL SUB=L13

FILE 'CAPLUS' ENTERED AT 12:19:03 ON 28 MAY 2003

L19               22 S L18  
L20               17 S L19 NOT PY>=2000

09/993,666

Page 1

=> d ibib ab hitstr 1-10

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:522625 CAPLUS  
 DOCUMENT NUMBER: 137:98953  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.: US 2000-235160P P 20000922				
OTHER SOURCE(S): MARPAT 137:98953				

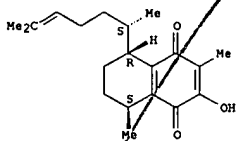
AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprising the administration of a pseudopterostin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. About 1.0 kg of P. elisabethae was freeze-dried and extd. with 600 ml of chloroform extns. The solvent was evapd. under reduced pressure to give 360 g of gum. This gum was then re-dissolved in 600 ml MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g of oil which chromatographed on a silica gel column to give various pseudopterostins, seco-pseudopterostins, and elisabethadiol. Pseudopterostins had high anti-inflammatory activity.

IT 433717-71-6, Elisabethadione  
 RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses) (anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (8R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:428919 CAPLUS  
 DOCUMENT NUMBER: 137:15779  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): The Regents of the University California, USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ; EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GN, GW, ML, MR, NE, SN, TD, TG

AU 2002041521 A5 20020611 AU 2002-41521 20011127  
 PRIORITY APPLN. INFO.: US 2000-253160P P 20001128  
 WO 2001-US44334 W 20011127

OTHER SOURCE(S): MARPAT 137:15779

AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. Examples are provided demonstrating the antiinflammatory, antiproliferative and analgesic activity of several compds. (pseudopterostin M, seco-pseudopterostin E, elisabethdione, etc.) isolated from P. elisabethae.

IT 433717-71-6P, Elisabethadione

RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pharmacol. activity of compds. derived from Pseudopterogorgia elisabethae)

RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (8R,8S)- (9CI) (CA INDEX NAME)

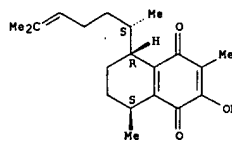
Absolute stereochemistry.

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

(Continued)

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS

(Continued)



09/993,666

Page 1

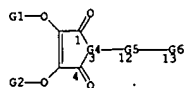
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L5 ANSWER 1 OF 2 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 129:175440 MARPAT  
 TITLE: Preparation of bicyclic quinones as mitochondrial function activators  
 INVENTOR(S): Kato, Kaneyoshi; Ohra, Taiichi; Miyamoto, Masaomi  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 224 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9833758	A1	19980806	WO 1998-JP422	19980202
V: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, YN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9856801	A1	19980825	AU 1998-56801	19980202
JP 10273469	A2	19981013	JP 1998-20100	19980202
EP 968164	A1	20000105	EP 1998-901088	19980202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6326369	B1	20011204	US 1999-341198	19990706
JP 1997-20763 19970203				
WO 1998-JP422 19980202				

PRIORITY APPLN. INFO.:  
 AB Title compds. [I; R1,R2 = alkyl; R1R2 = atoms to form a ring; R3R4 = atoms to form a (un)substituted ring having ZR as a substituent. R = (un)substituted OH, -NH2, -aryl, acyl; Z = 1-15 atom-contg. chain] were prepd. Thus, I (R1-R3 = Me, R4 = H) was converted in 4 steps to 1-bromo-6-bromomethyl-2,3,4,5-tetramethoxybenzene which was condensed with EtO2C(CH2)7CH(CO2Et)2 (prepn. given) to give, in 3 addnl. steps, I [R1 = R2 = Me, R3R4 = CH2CR5R6CH2, R5 = CO2Et, R6 = (CH2)7CO2Et]. Data for biol. activity of I were given.

MSTR 1A



G4 = 36-1 35-4 37-12

L5 ANSWER 2 OF 2 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 126:152798 MARPAT  
 TITLE: Tocotrienols and tocotrienol-like compounds and methods for their use  
 INVENTOR(S): Lane, Ronald H.; Qureshi, Asaf A.; Salser, Winston A.  
 PATENT ASSIGNEE(S): Lipogenics, Inc., USA  
 SOURCE: U.S., 41 pp., Cont.-in-part of U.S. Ser. No. 796,486, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5591772	A	19970107	US 1994-244215	19940815
WO 9309777	A1	19930527	WO 1992-US10277	19921120
V: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KR, LR, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9331502	A1	19930615	AU 1993-31502	19921120
AU 670557	B2	19960725		
JP 07504887	T2	19950601	JP 1992-509587	19921120
JP 2000169369	A2	20000620	JP 1999-332117	19921120
NO 9401929	A	19940713	NO 1994-1929	19940524
US 5908940	A	19990601	US 1996-583232	19960105
US 5821264	A	19981013	US 1996-719284	19960924
US 5919818	A	19990706	US 1997-991912	19971216
US 6143770	A	20001107	US 1998-182531	19981028
US 6204290	B1	20010320	US 1998-182384	19981028
US 6239171	B1	20010529	US 1998-182530	19981028

PRIORITY APPLN. INFO.:  
 AB The present invention relates to novel tocotrienols and tocotrienol-like compds. displaying biol. activity. The tocotrienols and tocotrienol-like compds. of this invention may be conveniently obtained from biol. sources or by chem. synthesis and may be used in pharmaceutical compns., foodstuffs and dietary supplements. This invention also relates to the use of tocotrienols, tocotrienol-like compds., and mixts. thereof, as hypocholesterolemic, antithrombotic, antioxidant, antiatherogenic, antiinflammatory, and immunoregulatory agents or as agents useful to decrease lipoprotein (a) concn. in the blood or to increase feed conversion efficiency.

MSTR 6

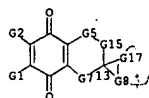
L5 ANSWER 1 OF 2 MARPAT COPYRIGHT 2003 ACS (Continued)



G5 = alkylene<(1-8)>  
 DER: or salts  
 MPL: claim 1

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 MARPAT COPYRIGHT 2003 ACS (Continued)



G1 = OH  
 G2 = OH  
 G5 = 26

HC—G6  
 26

G6 = alkyl<(1-6)>  
 G7 = 60

HC—G16  
 60

G15 = (0-4) CH2  
 DER: and salts, oxidation products and hydrolysis products  
 MPL: disclosure

=> d his

(FILE 'HOME' ENTERED AT 09:59:23 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 09:59:28 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

FILE 'BEILSTEIN' ENTERED AT 10:00:06 ON 28 MAY 2003

L4 0 S L1 FULL

FILE 'MARPAT' ENTERED AT 10:00:23 ON 28 MAY 2003

L5 2 S L2 FULL

=> d his

(FILE 'HOME' ENTERED AT 09:59:23 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 09:59:28 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

FILE 'BEILSTEIN' ENTERED AT 10:00:06 ON 28 MAY 2003

L4 0 S L1 FULL

FILE 'MARPAT' ENTERED AT 10:00:23 ON 28 MAY 2003

L5 2 S L2 FULL

FILE 'CAPLUS' ENTERED AT 10:04:56 ON 28 MAY 2003

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS

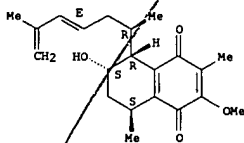
ACCESSION NUMBER: 2002:11433 CAPLUS  
 DOCUMENT NUMBER: 136:279574  
 TITLE: Total synthesis of colombiasin A and determination of its absolute configuration  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Chemistry--A European Journal (2001), 7(24), 5359-5371. CODEN: CEJUED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The total synthesis of the recently reported marine natural product colombiasin A (I) and detn. of its abs. configuration are reported. Two Diels-Alder cycloaddns. and a palladium-catalyzed rearrangement are employed as key reactions to construct the tetracyclic framework of the target mol. The enantioselective synthesis of colombiasin A utilizes Mikami's [(S)-BINOL-TiCl<sub>2</sub>] catalyst to asym. introduce the first chiral center during the initial Diels-Alder reaction and, in conjunction with X-ray crystallog. anal. of a bromine contg. deriv., led to the assignment of the abs. configuration of the natural product.

IT 362650-95-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A and detn. of its abs. configuration)

RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS

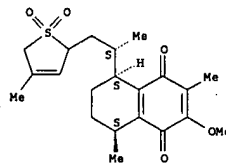
ACCESSION NUMBER: 2001:831849 CAPLUS  
 DOCUMENT NUMBER: 136:151319  
 TITLE: Towards colombiasin A  
 AUTHOR(S): Harrowven, David C.; Tyte, Melloney J.  
 CORPORATE SOURCE: Department of Chemistry, The University of Southampton, Southampton, SO17 1BJ, UK  
 SOURCE: Tetrahedron Letters (2001), 42(49), 8709-8711  
 CODEN: TETLEY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A synthetic route to an diastereomerically unnatural analog I of colombiasin A (II) is described. Key features are an arene alkylation with a .gamma.-methylene-.gamma.-butyrolactone and an intramol. Diels-Alder cycloaddn.

IT 394739-50-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthetic studies directed towards colombiasin A)

RN 394739-50-5 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, (5R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS

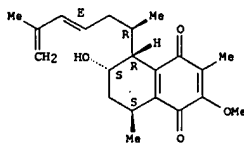
ACCESSION NUMBER: 2001:516801 CAPLUS  
 DOCUMENT NUMBER: 135:273093  
 TITLE: Total synthesis of Colombiasin A  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Angewandte Chemie, International Edition (2001), 40(13), 2482-2486  
 CODEN: ACHIEF; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:273093

AB The authors report the total synthesis of racemic colombiasin A (I) by a strategy which also delivered its C7 epimer as well as several other analogs.

IT 362650-95-1P 362651-05-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A)

RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

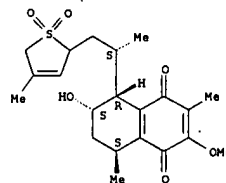
Relative stereochemistry.  
 Double bond geometry as shown.



RN 362651-05-6 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5S,6R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS (Continued)

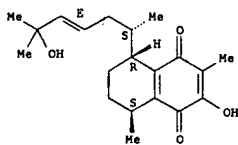


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



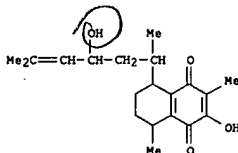
L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2000:895538 CAPLUS  
 DOCUMENT NUMBER: 134:160401  
 TITLE: Structurally diverse terpenoids from the sea whip *Pseudopterogorgia elisabethae* (Bayer)  
 AUTHOR(S): Rodriguez, A. D.; Shi, Y.-P.  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.  
 SOURCE: Tetrahedron (2000), 56(46), 9015-9023  
 CODEN: TETRAH; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The extn. of a specimen of *Pseudopterogorgia elisabethae* from Colombia afforded three new diterpenes (I-III), a norditerpene (IV), and a tetrasternoditerpene (V). Metabolites IV and V contain unusual carbon skeletons that are previously undescribed and therefore constitute new classes of C19 and C16 rearranged terpenes, resp. Full details of the isolation and structure elucidation of I-V, which were established by spectroscopic methods including comprehensive 2D NMR measurements, are provided herein.  
 IT 325691-48-3P  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (terpenoids from sea whip *Pseudopterogorgia elisabethae*)  
 RN 325691-48-3 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-[(1R,3E)-5-hydroxy-1,5-dimethyl-3-hexenyl]-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.  
 Double bond geometry as shown.  
 Currently available stereo shown.



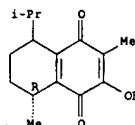
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1989:21335 CAPLUS  
 DOCUMENT NUMBER: 110:21335  
 TITLE: New marine diterpenoids, including a unique hydroperoxide, from a Caribbean gorgonian coral of the genus *Pseudopterogorgia*  
 AUTHOR(S): Harvis, Carl A.; Burch, Mark T.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Scripps Inst. Oceanogr., La Jolla, CA, 92093-0228, USA  
 SOURCE: Tetrahedron Letters (1988), 29(35), 4361-4  
 CODEN: TETLEA; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 110:21335  
 AB 4 New diterpenoids (I-IV) related to the aglycon components of the recently described pseudopterogins and seco-pseudopterogins have been isolated from an undescribed *Pseudopterogorgia* species from the Caribbean Sea. The new compds., described on the basis of their NMR properties and chem. interconversions, appear to be related, illustrating some interesting rearrangements of a tertiary hydroperoxide in this series.  
 IT 110169-36-1  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (of gorgonian coral)  
 RN 110169-36-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-(3-hydroxy-1,5-dimethyl-4-hexenyl)-3,8-dimethyl-, (9CI) (CA INDEX NAME)

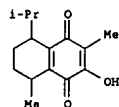


L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1998:108327 CAPLUS  
 DOCUMENT NUMBER: 128:192798  
 TITLE: Formation of mansonones from naturally occurring para-benzoquinones  
 AUTHOR(S): Garcia, Esther; Mendoza, Virgilio; Agustin Guzman, J.  
 CORPORATE SOURCE: Instituto Investigaciones Químico-Biológicas, Universidad Michoacana San Nicolás de Hidalgo, Morelia, 58030, Mex.  
 SOURCE: Natural Product Letters (1997), 11(1), 67-72  
 CODEN: NPLEEF; ISSN: 1057-5634  
 PUBLISHER: Harwood Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cyclization of perezene and hydroxyperezene with HI, followed by Jones oxidn., converted them into isomansonone A and mansonone A, B, and C.  
 IT 203174-32-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of mansonones from perezene)  
 RN 203174-32-7 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1967:105061 CAPLUS  
 DOCUMENT NUMBER: 66:105061  
 TITLE: Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Marini-Bettolo, Giovanni B.; Casinovi, Carlo G.; Galeffi, Corrado; Dalle Monache, Franco; Del Guercio, G.  
 CORPORATE SOURCE: Univ. Cattolica, Rome, Italy  
 SOURCE: Annali dell'Istituto Superiore di Sanita (1966), 2(2-3), 327-41  
 CODEN: AISSAW; ISSN: 0021-2571  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Italian  
 AB CA 64, 12728d. The wood of *M. altissima*, which is widely used for furniture making, was studied for the irritating and cardiokinetic substances it contains. By means of column chromatog., the crude CHCl<sub>3</sub> ext. of *M. altissima* was fractionated into 6 new quinones: red mansonone A (I), m. 117-18.degree., [α]<sub>D</sub> 200 680.degree. (c 0.2, CHCl<sub>3</sub>); gold-yellow mansonone B (II), m. 68-9.degree.; orange mansonone C (III), m. 134-8.degree.; orange mansonone D (IV), m. 173-5.degree.; orange-yellow mansonone E (V), m. 148-9.degree.; violet-mansonone F (VI), m. 214-15.degree.. Their structures were partially elucidated by chem. and spectroscopic analysis. A C15 skeleton which is a common feature for the compds. suggests a terpene origin. Two have the structure of oxaphenaleone and the 1st time in biflorin. I was easily reduced in H<sub>2</sub>O with Na hydroxysulfite. I was reduced with Zn in Ac<sub>2</sub>O and pyridine to yield the diacetate, m. 156-60.degree.. Ac<sub>2</sub>O and NaOAc yielded the acetate, b.p. 120.degree.. II, III, IV, and V were reduced by Na hydroxysulfite and reoxidized by air. III with pyridine, Ac<sub>2</sub>O, and Zn yielded the diacetate, m. 156-8.degree.. Boiling with an acetic acid soln. of o-phenylenediamine yielded the quinoxaline, m. 103-4.degree.. IV did not react with Ac<sub>2</sub>O and NaOAc. With Zn and Ac<sub>2</sub>O and pyridine it gave a diacetyl deriv. With o-phenylenediamine and acetate V gave a deriv., m. 148-50.degree.. With Zn, Ac<sub>2</sub>O, and pyridine V gave a diacetate, m. 110.degree.. VI is very sensitive to light and changes with time, especially in soln.  
 IT 14375-53-2  
 RL: PRP (Properties)  
 (structure of)  
 RN 14375-53-2 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67994 CAPLUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:127294-h, 12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of  
 Mansonia altissima  
 AUTHOR(S): Bettolo, G. B. Marini; Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: 1st. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE:

LANGUAGE: English

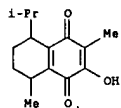
AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sep. the CHCl<sub>3</sub> irritative fraction into 6 C<sub>15</sub>-quinones designated as mansonones A, B, C, D, E, and F, m. 117-18.degree. (C<sub>6</sub>H<sub>12</sub>), 68-9.degree. (C<sub>6</sub>H<sub>14</sub>), 134-8.degree. (C<sub>6</sub>H<sub>14</sub>), 173-5.degree. (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>6</sub>), 148-9.degree. (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree. (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicronm.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -CH=CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C<sub>19</sub>H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicronm.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b<sub>0</sub>.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, alc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formulas is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Sandermann and Dietrichs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicronm.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

IT 14375-53-2, Mansonone B

(structure of)

RN 14375-53-2 CAPLUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS (Continued)

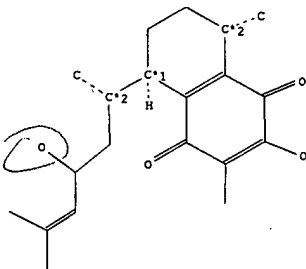
09/993,666

Page 6

=> d all 1-2

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 5095107  
 Beilstein Pref. RN (BPR): 118169-36-1  
 CAS Reg. No. (RN): 118169-36-1  
 Chemical Name (CN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Autonom Name (AUN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molec. Formula (MF): C20 H28 O4  
 Molecular Weight (MW): 332.44  
 Lawson Number (LN): 9791  
 File Segment (FS): relative configuration, Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 4527263  
 Tautomer ID (TAUTID): 4874682  
 Beilstein Citation (BSO): 6-08  
 Entry Date (DED): 1992/08/28  
 Update Date (DUPD): 1993/03/20



## Atom/Bond Notes:

1. CIP Descriptor: R
  2. CIP Descriptor: S
- Fragment Notes:  
 Alternatively represents mirror image  
 Stereo Descriptor: rel

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

1. 3000 - 1640 cm<sup>-1</sup> (-1)

## UV and Visible Spectrum:

Description	Solvent	Absorption	Ext./Abs. Coeff.	Ref.
(.KW)	(.SOL)	Maxima	(.EAC)	
		(.AN)	(1/MOL*CM)	
Absorption maxima	methanol	326, 281, 223	4600, 7500, 15700	1
Absorption maxima	methanol	321, 279, 220	3100, 8900, 13200	1

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

BPR Beilstein Preferred RN 1  
 RN CAS Registry Number 1  
 CN Chemical Name 1  
 AUN Autonomname 1  
 MF Molecular Formula 1  
 FW Formular Weight 1  
 LN Lawson Number 1  
 FS File Segment 2  
 CTYPE Compound Type 1  
 CONSID Constitution ID 1  
 TAUTID Tautomer ID 1  
 BSO Beilstein Citation 1  
 ED Entry Date 1  
 UPD Update Date 1  
 INP Isolation from Natural Product 1  
 IR Infrared Spectrum 1  
 NMR Nuclear Magnetic Resonance 2  
 UVS UV and Visible Spectrum 2

## Isolation from Natural Product:

INF

(INP): Pseudopterogorgia

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts  
 Nucleus (.NUC): 1H  
 Solvents (.SOL): CDCl3

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

NMR

Description (.KW): Chemical shifts  
 Nucleus (.NUC): 13C  
 Solvents (.SOL): benzene-d6

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Infrared Spectrum:

Description	Solvent	Ref.	Note
ion			
(.KW)	(.SOL)		
Bands	CHCl3	1	1

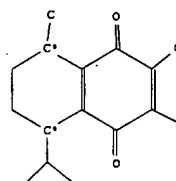
## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Notes(s):

## L8 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 2053092  
 Beilstein Pref. RN (BPR): 14375-53-2  
 CAS Reg. No. (RN): 14375-53-2  
 Chemical Name (CN): Mansonon B  
 Autonom Name (AUN): 2-hydroxy-5-isopropyl-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molec. Formula (MF): C15 H20 O3  
 Molecular Weight (MW): 248.32  
 Lawson Number (LN): 9296  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 1884852  
 Tautomer ID (TAUTID): 2003770  
 Beilstein Citation (BSO): 5-08  
 Entry Date (DED): 1989/06/29  
 Update Date (DUPD): 1992/06/02



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
INP	Isolation from Natural Product	2
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1
RSTR	Related Structure	1
UVS	UV and Visible Spectrum	1

## Related Structure:

L8 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

RSTR

## Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

## Isolation from Natural Product:

INP

(INP): M. altissima

## Reference(s):

1. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAW, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

INP

(INP): a. Mansonia Altissima Cher.

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

## Melting Point:

Value (Ref.

(MP) |

(Cel) |

-----|-----

68 - 69 | 1, 2

## Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857
2. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAW, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

## Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts

## Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

## UV and Visible Spectrum:

Description (Ref.

(.KW) |

-----|-----

Absorption maxima | 1

## Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

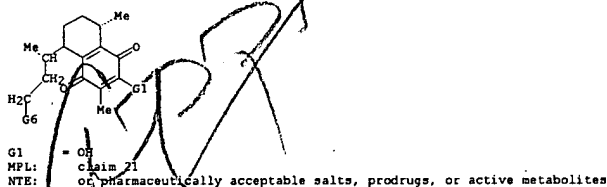
=> d ibib ab fqhit 1-3

L9 ANSWER 1 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 137:98953 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
*Pseudopterogorgia elisabethae*  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.:			US 2000-235160P	20000922

AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprising the administration of a pseudopterogorgia (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH<sub>2</sub>OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterogorgia and compds. related to pseudopterogorgia are disclosed. About 1.0 kg *P. elisabethae* was freeze-dried and extd. with MeOH and followed with 2 Chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 600 ml MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl<sub>3</sub> to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterogorgia, seco-pseudopterogorgia, and elisabethadiol. Pseudopterogorgia had high anti-inflammatory activity.

MYR 3



L9 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS (Continued)  
 G1 = OH  
 MPL: claim 21  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L9 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 137:15779 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
*Pseudopterogorgia elisabethae*  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): The Regents of the University California, USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

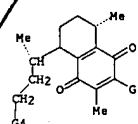
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MW, MX, MY, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AA, AB, AC, AD, AE, AF, AG, AH, AI, AJ, AK, AL, AM, AN, AO, AP, AQ, AR, AS, AT, AU, AV, AW, AX, AY, AZ, BA, BB, BC, BD, BE, BF, BJ, BK, BL, BM, BN, BO, BP, BQ, BR, BS, BT, BU, BV, BW, BY, BZ, CA, CB, CC, CD, CE, CF, CG, CH, CI, CJ, CK, CL, CM, CN, CO, CP, CQ, CR, CS, CT, CU, CV, CW, CX, CY, CZ, DA, DB, DD, DE, DF, DG, DH, DI, DJ, DK, DL, DM, DN, DO, DP, DQ, DR, DS, DT, DU, DV, DW, DX, DY, DZ, EA, EB, EC, ED, EE, EF, EG, EH, EI, EJ, EK, EL, EM, EN, EO, EP, EQ, ER, ES, ET, EU, EV, EW, EX, EY, EZ, FA, FB, FC, FD, FE, FF, FG, FH, FI, FJ, FK, FL, FM, FN, FO, FP, FQ, FR, FS, FT, FU, FV, FW, FX, FY, FZ, GA, GB, GC, GD, GE, GF, GG, GH, GI, GJ, GK, GL, GM, GN, GP, GQ, GR, GS, GT, GU, GV, GW, GX, GY, GZ, HA, HB, HC, HD, HE, HF, HG, HH, HI, HJ, HK, HL, HM, HN, HO, HP, HQ, HR, HS, HT, HU, HV, HW, HX, HY, HZ, IA, IB, IC, ID, IE, IF, IG, IH, II, IJ, IK, IL, IM, IN, IO, IP, IQ, IR, IS, IT, IU, IV, IW, IX, IY, IZ, JA, JB, JC, JD, JE, JF, JG, JH, JI, JJ, JK, JL, JM, JN, JO, JP, JQ, JR, JS, JT, JU, JV, JW, JX, JY, JZ, KA, KB, KC, KD, KE, KF, KG, KH, KI, KJ, KK, KL, KM, KN, KO, KP, KQ, KR, KS, KT, KU, KV, KW, KX, KY, KZ, LA, LB, LC, LD, LE, LF, LG, LH, LI, LJ, LK, LM, LN, LO, LP, LQ, LR, LS, LT, LU, LV, LW, LX, LY, LZ, MA, MB, MC, MD, ME, MF, MG, MH, MI, MJ, MK, ML, MN, MO, MP, MQ, MR, MS, MT, MU, MV, MW, MX, MY, MZ, NA, NB, NC, ND, NE, NF, NG, NH, NI, NJ, NK, NL, NM, NO, NP, NQ, NR, NS, NT, NU, NV, NW, NX, NY, NZ, OA, OB, OC, OD, OE, OF, OG, OH, OI, OJ, OK, OL, OM, ON, OO, OP, OQ, OR, OS, OT, OU, OV, OW, OX, OY, OZ, PA, PB, PC, PD, PE, PF, PG, PH, PI, PJ, PK, PL, PM, PN, PO, PP, PQ, PR, PS, PT, PU, PV, PW, PX, PY, PZ, QA, QB, QC, QD, QE, QF, QG, QH, QI, QJ, QK, QL, QM, QN, QO, QP, QQ, QR, QS, QT, QU, QV, QW, QX, QY, QZ, RA, RB, RC, RD, RE, RF, RG, RH, RI, RJ, RK, RL, RM, RN, RO, RP, RQ, RR, RS, RT, RU, RV, RW, RX, RY, RZ, SA, SB, SC, SD, SE, SF, SG, SH, SI, SJ, SK, SL, SM, SN, SO, SP, SQ, SR, SS, ST, SU, SV, SW, SX, SY, SZ, TA, TB, TC, TD, TE, TF, TG, TH, TI, TJ, TK, TL, TM, TN, TO, TP, TQ, TR, TS, TT, TU, TV, TW, TX, TY, TZ, UA, UB, UC, UD, UE, UF, UG, UH, UI, UJ, UK, UL, UM, UN, UO, UP, UQ, UR, US, UT, UU, UV, UW, UX, UY, UZ, VA, VB, VC, VD, VE, VF, VG, VH, VI, VJ, VK, VL, VM, VN, VO, VP, VQ, VR, VS, VT, VU, VV, VW, VX, VY, VZ, WA, WB, WC, WD, WE, WF, WG, WH, WI, WJ, WK, WL, WM, WN, WO, WP, WQ, WR, WS, WT, WU, WV, WX, WY, WZ, XA, XB, XC, XD, XE, XF, XG, XH, XI, XJ, XK, XL, XM, XN, XO, XP, XQ, XR, XS, XT, XU, XV, XW, XX, XY, XZ, YA, YB, YC, YD, YE, YF, YG, YH, YI, YJ, YK, YL, YM, YN, YO, YP, YQ, YR, YS, YT, YU, YV, YW, YX, YY, YZ, ZA, ZB, ZC, ZD, ZE, ZF, ZG, ZH, ZI, ZJ, ZK, ZL, ZM, ZN, ZO, ZP, ZQ, ZR, ZS, ZT, ZU, ZV, ZW, ZX, ZY, ZZ.

AU 2002041521 A5 20020611 AU 2002-41521 20011127  
 PRIORITY APPLN. INFO.:

AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH<sub>3</sub>, or CH<sub>2</sub>OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterogorgia and compds. related to pseudopterogorgia are disclosed. Examples are provided demonstrating the anti-inflammatory, antiproliferative and analgesic activity of several compds. (pseudopterogorgia M, seco-pseudopterogorgia E, elisabethdione, etc.) isolated from *P. elisabethae*.

MYR 3



L9 ANSWER 3 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 110:4187 MARPAT  
 TITLE: Composition and method for rapid differentiation of  
 viable fungi from bacteria using polyene antibiotics  
 Cichanowicz, Peggy Woodruff; Belly, Robert Troconis  
 PATENT ASSIGNEE(S): Eastman Kodak Co., USA  
 SOURCE: Eur. Pat. Appl., 22 pp.  
 CODEN: EPOXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 261931	A2	19880330	EP 1987-308380	19870922
EP 261931	A3	19891011		

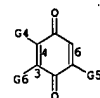
R: CH, DE, FR, GB, LI  
 CA 1290226 A1 19911008 CA 1986-523203 19861118  
 PRIORITY APPLN. INFO.:

AB Viable fungi are rapidly differentiated from viable bacteria by incubation with a compn. contg. a polyene antibiotic which affects membrane function in fungi and a compd. [e.g. a RIND compd. (reducible compd. which undergoes intramol. nucleophilic displacement) such as quinone I, where R1 = (R5)m(R6)QX; R2, R4 = H, (substituted) alkyl or aryl, electron-withdrawing group; R3 = R1, R2; or R3R4 complete a (substituted) strained fused carbocyclic ring; R5 = (substituted) C1-2 alkyls; R6 = (substituted) alkyl, cycloalkyl, aryl, or heterocycle; Q = C(O), C(S); X = shiftable detectable species which provides a detectable species when released; m = 0, 1] which is normally reducible by both fungi and bacteria. The antibiotic selectively inhibits the redn. of the reducible compd. by the fungi but does not affect the reducing capacity of the bacteria. A soln. contg. RIND compd. II, glucose, trimethyl-1,4-benzoquinone (electron transfer agent), buffer, and filipin (polyene antibiotic) at various dilns. was incubated with suspensions of various bacteria and fungi at 37 degree for 30 min, and the difference in relative fluorescence before and after incubation was measured with excitation at 540 nm and emission at 620 nm. The percent inhibition of redn. of II at 0.52 mg filipin/ml was: *Escherichia coli*, 0; *Staphylococcus aureus*, 8.6; *Candida albicans*, 71.0; *Aspergillus flavus*, 42.5.

MYR 18

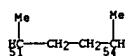
G2-G1

G1 = 6



G5 = OMe  
 G7 = alkylene<(1-2)> (SO (1-) G11)  
 G4 + G6 = 51-4 54-3

L9 ANSWER 3 OF 3 HARPAT COPYRIGHT 2003 ACS (Continued)



MPL: claim 4



## L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67994 CAPLUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:12728d-h, 12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Bettolo, G. B.; Marini, Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: 1st. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extrn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sep'd. the CHCl<sub>3</sub> irritative fraction into 6 C15-quinones designated as mansonones A, B, C, D, E, and F, m. 117-18.degree. (C<sub>6</sub>H<sub>12</sub>), 68-9.degree. (C<sub>6</sub>H<sub>14</sub>), 134-8.degree. (C<sub>6</sub>H<sub>14</sub>), 173-5.degree. (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>5</sub>), 148-9.degree. (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree. (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -CMe:CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C<sub>19</sub>H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b0.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, alc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formulae is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Syndermann and Districhs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

## L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67993 CAPLUS  
 DOCUMENT NUMBER: 64:67993  
 ORIGINAL REFERENCE NO.: 64:12728c-d  
 TITLE: Terpenoid chemistry. XI. (-)-.beta.-Sesquiphellandrene  
 AUTHOR(S): Connell, D. W.; Sutherland, M. D.  
 CORPORATE SOURCE: Univ. Queensland, Brisbane  
 SOURCE: Australian Journal of Chemistry (1966), 19(2), 283-8  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB cf. CA 62, 5301a; 63, 14915f. A new natural sesquiterpene, (-)-.beta.-sesquiphellandrene (I), b1 90-0.5.degree., n<sub>D</sub><sup>25</sup> 1.4973, d<sub>25</sub> 0.8760, [.alpha.]<sub>D</sub><sup>20</sup> -3.99.degree. (neat), has been isolated from ginger oil in .apprx.96% purity (principal impurity (-)-.beta.-bisabolene) by distn. and gas chromatography on AgNO<sub>3</sub>-treated alumina. Rel. retentions for I on Apiezon M, butanediol succinate polyester, castor wax, and cyanosilicone (KF 1150) at 130-85.degree. are given with respect to caryophyllene, humulene, and zingiberene. On hydrogenation I yields bisabolene; reaction with anhyd. HCl in AcOH gives isozingiberene-2HCl. I nitrosite, m. 88-90.degree. (decompn.), [.alpha.]<sub>D</sub><sup>20</sup> 29.degree. (c 1.5, CHCl<sub>3</sub>), forms with NaN<sub>2</sub>. I forms a Diels-Alder adduct with p-phenylazophenylmaleinanal in the presence (but not in the absence) of (CO<sub>2</sub>H)<sub>2</sub>, m. 142.degree., [.alpha.]<sub>D</sub><sup>24</sup> -222.degree. (hexane).

=> d his

(FILE 'HOME' ENTERED AT 10:46:53 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 10:47:14 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 9 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 28 MAY 2003

L4 10 S L3

FILE 'USPATFULL' ENTERED AT 10:53:47 ON 28 MAY 2003

L5 1 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 10:54:35 ON 28 MAY 2003

L7 2 S L3

L8 2 S L3 FULL

FILE 'MARPAT' ENTERED AT 10:55:51 ON 28 MAY 2003

L9 3 S L3 FULL

=> d ibib ab 1-2

=> d his

(FILE 'HOME' ENTERED AT 10:46:53 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 10:47:14 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 9 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 28 MAY 2003

L4 10 S L3

FILE 'USPATFULL' ENTERED AT 10:53:47 ON 28 MAY 2003

L5 1 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 10:54:35 ON 28 MAY 2003

L7 2 S L3

L8 2 S L3 FULL

FILE 'MARPAT' ENTERED AT 10:55:51 ON 28 MAY 2003

L9 3 S L3 FULL

FILE 'CAOLD' ENTERED AT 10:58:13 ON 28 MAY 2003

L10 1 S L3

SEL AN 1-

FILE 'CAPLUS' ENTERED AT 10:58:29 ON 28 MAY 2003

L11 2 S E1/OREF

L19 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2003 ACS

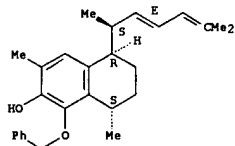
ACCESSION NUMBER: 1998:736134 CAPLUS  
 DOCUMENT NUMBER: 130:95692  
 TITLE: A Direct and Efficient Stereocontrolled Synthetic Route to the Pseudo-terpenes, Potent Marine Anti-inflammatory Agents  
 AUTHOR(S): Corey, E. J.; Lazerwith, Scott E.  
 CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA  
 SOURCE: Journal of the American Chemical Society (1998), 120(49), 12777-12782  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 130:95692

AB Described herein is a new synthetic route to pseudo-terpenes aglycon (I), a key intermediate for the synthesis of a group of anti-inflammatory natural products including pseudo-terpenes A and E. The pathway of synthesis starts with the abundant and inexpensive (S)-(-)-limonene and its long-known cyclic hydroboration product (II) and leads to the chiral hydroxy ketone (III). Conversion of III to (IV) followed by a novel arom. annulation produced (V) which underwent a highly diastereoselective cyclization to afford the protected pseudo-terpenes aglycon (VI). The naturally occurring pseudo-terpenes A and E are readily available from this key intermediate.

IT 219498-24-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (stereoselective synthesis of pseudo-terpenes aglycon)

RN 219498-24-5 CAPLUS  
 CN 2-Naphthalenol, 5-[(1S,2E)-1,5-dimethyl-2,4-hexadienyl]-5,6,7,8-tetrahydro-3,8-dimethyl-1-(phenylmethoxy)-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
 Double bond geometry, as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

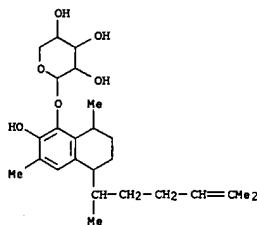
L19 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:749996 CAPLUS  
 DOCUMENT NUMBER: 128:34906  
 TITLE: Enantioselective synthesis of the aglycons of pseudo-terpenes A and seco-pseudo-terpenes A via a common synthetic intermediate  
 AUTHOR(S): Majdalani, Andre; Schmalz, Hans Guenther  
 CORPORATE SOURCE: Institut Organische Chemie, Technische Universitaet Berlin, Berlin, D-10623, Germany  
 SOURCE: Synlett (1997), (11), 1303-1305  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A synthesis proceeding in 12 steps from the chiral building block I to the key intermediate II (R = SO<sub>2</sub>Ph) from which both the title compds. are easily accessible in 2 steps is reported.

IT 111466-65-0P, Secopseudo-terpenes A  
 RL: PMU (Preparation, unclassified); PREP (Preparation)  
 (stereoselective synthesis of pseudo-terpenes and seco-pseudo-terpenes aglycons)

RN 111466-65-0 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)



IT 199439-75-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (stereoselective synthesis of pseudo-terpenes and seco-pseudo-terpenes aglycons)

RN 199439-75-3 CAPLUS  
 CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L19 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2003 ACS

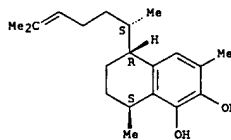
ACCESSION NUMBER: 1998:159578 CAPLUS  
 DOCUMENT NUMBER: 128:230537  
 TITLE: Preparation of heliopodin D from the seco-pseudo-terpenes aglycon: revision of the stereostructure of heliopodin D  
 AUTHOR(S): Geller, Thomas; Jakupovic, Jasmin; Schmalz, Hans-Gunther  
 CORPORATE SOURCE: Institut fur Organische Chemie der Technischen Universitaet, Berlin, D-10623, Germany  
 SOURCE: Tetrahedron Letters (1998), 39(12), 1541-1544  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A revised stereostructure for heliopodin D (I) was unequivocally established by its synthesis from the seco-pseudo-terpenes aglycon and by careful anal. of NMR data. As the corresponding benzodioxole derived from the pseudo-terpenes A aglycon was not identical with heliopodin E, it was proven that heliopodin D and E do not belong to the same stereochem. series.

IT 199439-75-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. and revision of stereostructure of heliopodin D)

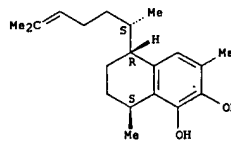
RN 199439-75-3 CAPLUS  
 CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



09/993,666

Page 1

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L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:522625 CAPLUS  
 DOCUMENT NUMBER: 137:98953  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.:		US 2000-235160P P 20000922		

OTHER SOURCE(S): MARPAT 137:98953

AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprise the administration of a pseudopterostin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 60% aq. MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterostins, seco-pseudopterostins, and elisabethadiol. Pseudopterostins had high anti-inflammatory activity.

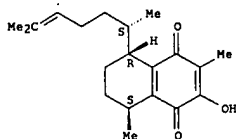
IT 433717-71-6, Elisabethadione

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses) (anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:428919 CAPLUS  
 DOCUMENT NUMBER: 137:15779  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): The Regents of the University California, USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXX02  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 AU 2002041521 A5 20020611 AU 2002-41521 20011127

PRIORITY APPLN. INFO.: US 2000-253160P P 20001128  
 WO/2001-US44334 W 20011127

OTHER SOURCE(S): MARPAT 137:15779

AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. Examples are provided demonstrating the antiinflammatory, antiproliferative and analgesic activity of several compds. (pseudopterostin M, seco-pseudopterostin E, elisabethadione, etc.) isolated from P. elisabethae.

IT 433717-71-6P, Elisabethadione

RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pharmacol. activity of compds. derived from Pseudopterogorgia elisabethae)

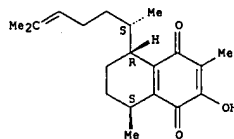
RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS (Continued)

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS (Continued)



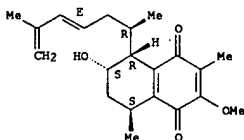
L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2002:11433 CAPLUS  
 DOCUMENT NUMBER: 136:279574  
 TITLE: Total synthesis of colombiasin A and determination of its absolute configuration  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Chemistry--A European Journal (2001), 7(24), 5359-5371  
 CODEN: CEUJED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The total synthesis of the recently reported marine natural product colombiasin A (I) and detn. of its abs. configuration are reported. Two Diels-Alder cycloaddns. and a palladium-catalyzed rearrangement are employed as key reactions to construct the tetracyclic framework of the target mol. The enantioselective synthesis of colombiasin A utilizes Mikami's [(S)-BINOL-TiCl<sub>2</sub>] catalyst to asym. introduce the first chiral center during the initial Diels-Alder reaction and, in conjunction with X-ray crystallog. anal. of a bromine contg. deriv., led to the assignment of the abs. configuration of the natural product.

IT 362650-95-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A and detn. of its abs. configuration)

RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

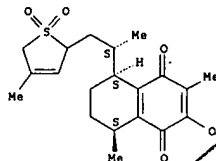
L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2001:631849 CAPLUS  
 DOCUMENT NUMBER: 136:151319  
 TITLE: Towards colombiasin A  
 AUTHOR(S): Harrowven, David C.; Tyte, Melloney J.  
 CORPORATE SOURCE: Department of Chemistry, The University of Southampton, Southampton, SO17 1BJ, UK  
 SOURCE: Tetrahedron Letters (2001), 42(49), 8709-8711  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A synthetic route to an diastereomerically unnatural analog I of colombiasin A (II) is described. Key features are an arene alkylation with a .gamma.-methylene-.gamma.-butyrolactone and an intramol. Diels-Alder cycloaddn.

IT 394739-50-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthetic studies directed towards colombiasin A)

RN 394739-50-5 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, (5R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

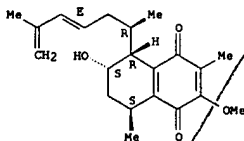
L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2001:516801 CAPLUS  
 DOCUMENT NUMBER: 135:273093  
 TITLE: Total synthesis of Colombiasin A  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Angewandte Chemie, International Edition (2001), 40(13), 2482-2486  
 CODEN: ACHIEF; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:273093

AB The authors report the total synthesis of racemic colombiasin A (I) by a strategy which also delivered its C7 epimer as well as several other analogs.

IT 362650-95-1P 362651-05-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A)

RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

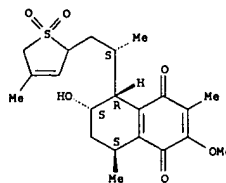
Relative stereochemistry.  
 Double bond geometry as shown.



RN 362651-05-6 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5S,6R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS (Continued)

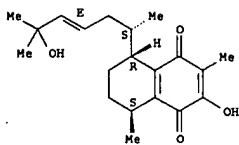


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:895538 CAPLUS  
 DOCUMENT NUMBER: 134:160401  
 TITLE: Structurally diverse terpenoids from the sea whip *Pseudopterogorgia elisabethae* (Bayer)  
 AUTHOR(S): Rodriguez, A. D.; Shi, Y.-P.  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.  
 SOURCE: Tetrahedron (2000), 56(46), 9015-9023  
 CODEN: TETRA; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The extra. of a specimen of *Pseudopterogorgia elisabethae* from Colombia afforded three new diterpenes (I-III), a norditerpene (IV), and a tetrasternoditerpene (V). Metabolites IV and V contain unusual carbon skeletons that are previously undescribed and therefore constitute new classes of C19 and C16 rearranged terpenes, resp. Full details of the isolation and structure elucidation of I-V, which were established by spectroscopic methods including comprehensive 2D NMR measurements, are provided herein.  
 IT RI: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (terpenoids from sea whip *Pseudopterogorgia elisabethae*)  
 RN 325691-48-3 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-[(1R,3E)-5-hydroxy-1,5-dimethyl-3-hexenyl]-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

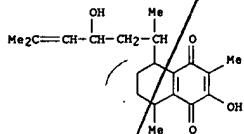
Rotation (+). Absolute stereochemistry unknown.  
 Double bond geometry as shown.  
 Currently available stereo shown.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS

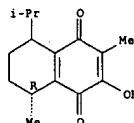
ACCESSION NUMBER: 1989:21335 CAPLUS  
 DOCUMENT NUMBER: 110:21335  
 TITLE: New marine diterpenoids, including a unique hydroperoxide, from a Caribbean gorgonian coral of the genus *Pseudopterogorgia*  
 AUTHOR(S): Harvis, Carl A.; Burch, Mark T.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Scripps Inst. Oceanogr., La Jolla, CA, 92093-0228/ USA  
 SOURCE: Tetrahedron Letters (1988), 29(35), 4361-4  
 CODEN: TETRA; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 110:21335  
 AB 4 New diterpenoids (I-IV) related to the aglycon components of the recently described pseudopterogins and seco-pseudopterogins have been isolated from an undescribed *Pseudopterogorgia* species from the Caribbean Sea. The new compds., described on the basis of their NMR properties and chem. interconversions, appear to be related, illustrating some interesting rearrangements of a tertiary hydroperoxide in this series.  
 IT 118169-36-1  
 RI: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (of gorgonian coral)  
 RN 118169-36-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-(3-hydroxy-1,5-dimethyl-4-hexenyl)-3,8-dimethyl-, (9CI) (CA INDEX NAME)



## L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS

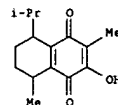
ACCESSION NUMBER: 1998:108327 CAPLUS  
 DOCUMENT NUMBER: 128:192798  
 TITLE: Formation of mansonones from naturally occurring para-benzoquinones  
 AUTHOR(S): Garcia, Esther; Mendoza, Virgilio; Agustin Guzman, J.  
 CORPORATE SOURCE: Instituto Investigaciones Químico-Biológicas, Universidad Michoacana San Nicolás de Hidalgo, Morelia, 58030, Mex.  
 SOURCE: Natural Product Letters (1997), 11(1), 67-72  
 CODEN: NPLEEF; ISSN: 1057-5634  
 PUBLISHER: Harwood Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cyclization of perezone and hydroxyperezone with HI, followed by Jones oxidn., converted them into isomansonone A and mansonone A, B, and C.  
 IT 203174-32-7P  
 RI: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of mansonones from perezone)  
 RN 203174-32-7 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-bis(methyl-5-(1-methylethyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



## L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1967:105061 CAPLUS  
 DOCUMENT NUMBER: 66:105061  
 TITLE: Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Marini-Bettolo, Giovanni B.; Casinovi, Carlo G.; Galeffi, Corrado; Delle Monache, Franco; Del Guercio, G.  
 CORPORATE SOURCE: Univ. Cattolica, Rome, Italy  
 SOURCE: Annali dell'Istituto Superiore di Sanita (1966), 2(2-3), 327-41  
 CODEN: AISSAW; ISSN: 0021-2571  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Italian  
 AB CA 64, 12728d. The wood of *M. altissima*, which is widely used for furniture making, was studied for the irritating and cardiokinetic substances it contains. By means of column chromatog., the crude CHC13 ext. of *M. altissima* was fractionated into 6 new quinones: red mansonone A (I), m. 117-18.degree., (.alpha.)200 680.degree., (c 0.2, CHC13); gold-yellow mansonone B (II), 68-9.degree., orange mansonone C (III), m. 134-8.degree., orange mansonone D (IV), m. 173-5.degree., orange-yellow mansonone E (V), m. 148-9.degree., violet-mansonone F (VI), m. 214-15.degree.. Their structures were partially elucidated by chem. and spectroscopic analysis. A C15 skeleton which is a common feature for the compds. suggests a terpene origin. Two have the structure of oxaphenaleone found the 1st time in biflorin. I was easily reduced in H2O with Na hydrosulfite. I was reduced with Zn in Ac2O and pyridine to yield the diacetate, m. 158-60.degree.. Ac2O and NaOAc yielded the acetate, b.p. 0.2 120.degree.. II, III, IV, and V were reduced by Na hydrosulfite and reoxidized by air. III with pyridine, Ac2O, and Zn yielded the diacetate, m. 156-8.degree.. Boiling with an acetic acid soln. of o-phenylenediamine yielded the quinoxaline, m. 103-4.degree.. IV did not react with Ac2O and NaOAc. With Zn and Ac2O and pyridine it gave a diacetyl deriv. With o-phenylenediamine and acetate V gave a deriv., m. 148-50.degree.. With Zn, Ac2O, and pyridine V gave a diacetate, m. 110.degree.. VI is very sensitive to light and changes with time, especially in soln.  
 IT 14375-53-2  
 RI: PRP (Properties)  
 (structure of)  
 RN 14375-53-2 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)





L4 ANSWER 10 OF 10 CAPIUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67994 CAPIUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:12728d-h,12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of *Mansononia altissima*  
 AUTHOR(S): Bettolo, G. B. Marini; Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: 1st. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

L4 ANSWER 10 OF 10 CAPIUS COPYRIGHT 2003 ACS (Continued)

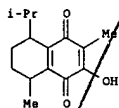
AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sep'd. the CHCl<sub>3</sub> irritative fraction into 6 C15-quinones designated as mansonones A, B, C, D, E, and F, m. 117-18.degree. (C<sub>6</sub>H<sub>12</sub>), 68-9.degree. (C<sub>6</sub>H<sub>14</sub>), 134-8.degree. (C<sub>6</sub>H<sub>14</sub>), 173-5.degree. (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>6</sub>), 148-9.degree. (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree. (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicronm.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -OMe:CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C<sub>19</sub>H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicronm.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b0.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, alc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formula is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Sandermann and Dietrichs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicronm.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

IT 14375-53-2, Mansonone B

(structure of)

RN 14375-53-2 CAPIUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl) (9CI) (CA INDEX NAME)



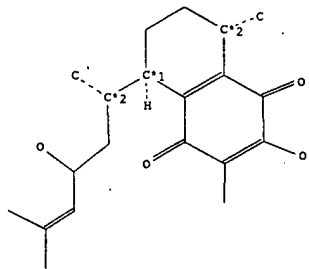
09/993,666

Page 6

=> d all 1-2

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 5095107  
 Beilstein Pref. RN (BPR): 118169-36-1  
 CAS Reg. No. (RN): 118169-36-1  
 Chemical Name (CN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Autonom Name (AUN): 2-hydroxy-5-(3-hydroxy-1,5-dimethyl-hex-4-enyl)-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molac. Formula (MF): C20 H28 O4  
 Molecular Weight (MW): 332.44  
 Lawson Number (LN): 9791  
 File Segment (FS): relative configuration, Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 4527263  
 Tautomer ID (TAUTID): 4874682  
 Beilstein Citation (BSO): 6-08  
 Entry Date (DED): 1992/08/28  
 Update Date (DUPD): 1993/03/20



Atom/Bond Notes:  
 1. CIP Descriptor: R  
 2. CIP Descriptor: S  
 Fragment Notes:  
 Alternatively represents mirror image  
 Stereo Descriptor: rel

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

1. 3000 - 1640 cm<sup>-1</sup>(-1)

## UV and Visible Spectrum:

Description	Solvent	Absorption	Ext./Abs. Coeff.	Ref.
(.KW)	(.SOL)	Maxima	(.EAC)	
		(nm)	(l/MOL*CM)	
Absorption maxima (methanol)		326, 281, 223	4600, 7500, 15700	1
Absorption maxima (methanol)		321, 279, 220	3100, 8900, 13200	1

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## L8 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

BPR Beilstein Preferred RN 1  
 RN CAS Registry Number 1  
 CN Chemical Name 1  
 AUN Autonomname 1  
 MF Molecular Formula 1  
 FW Formular Weight 1  
 LN Lawson Number 1  
 FS File Segment 2  
 CTYPE Compound Type 1  
 CONSID Constitution ID 1  
 TAUTID Tautomer ID 1  
 BSO Beilstein Citation 1  
 ED Entry Date 1  
 UPD Update Date 1  
 INP Isolation from Natural Product 1  
 IR Infrared Spectrum 1  
 NMR Nuclear Magnetic Resonance 2  
 UVS UV and Visible Spectrum 2

## Isolation from Natural Product:

INP

(INP): Pseudopterogorgia

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts

Nucleus (.NUC): <sup>1</sup>HSolvents (.SOL): CDCl<sub>3</sub>

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

NMR

Description (.KW): Chemical shifts

Nucleus (.NUC): <sup>13</sup>CSolvents (.SOL): benzene-d<sub>6</sub>

## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Infrared Spectrum:

Description	Solvent	Ref.	Note
ion			
(.KW)	(.SOL)		
Bands	CHCl <sub>3</sub>	1	1

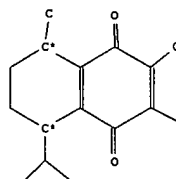
## Reference(s):

1. Harvis, Carl A.; Burch, Mark T.; Fenical, William, Tetrahedron Lett., CODEN: TELEAY, 29(35), <1988>, 4361-4364; BABS-5612346

## Notes(s):

## L8 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 2053092  
 Beilstein Pref. RN (BPR): 14375-53-2  
 CAS Reg. No. (RN): 14375-53-2  
 Chemical Name (CN): Mansonon B  
 Autonom Name (AUN): 2-hydroxy-5-isopropyl-3,8-dimethyl-5,6,7,8-tetrahydro-  
 <1,4>naphthoquinone  
 Molac. Formula (MF): C15 H20 O3  
 Molecular Weight (MW): 248.32  
 Lawson Number (LN): 9296  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 1884852  
 Tautomer ID (TAUTID): 2003770  
 Beilstein Citation (BSO): 5-08  
 Entry Date (DED): 1989/06/29  
 Update Date (DUPD): 1992/06/02



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
INP	Isolation from Natural Product	2
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1
RSTR	Related Structure	1
UVS	UV and Visible Spectrum	1

## Related Structure:

L8 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

RSTR

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

Isolation from Natural Product:

INP

(INP): M. altissima

Reference(s):

1. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAV, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

INP

(INP): a. Mansonia Altissima Cher.

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

Melting Point:

Value | Ref.

(MP) |

(Cel) |

-----|-----

68 - 69 | 1, 2

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857
2. Marini-Bettolo et al., Ann.Ist.Super.Sanita, CODEN: AISSAV, 2(2-3), <1966>, 327,328-341, Chem.Abstr., 66(105061), <1967>

Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

UV and Visible Spectrum:

Description | Ref.

(.KW) |

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Absorption maxima | 1

Reference(s):

1. Bettolo et al., Tetrahedron Lett., CODEN: TELEAY, <1965>, 4857

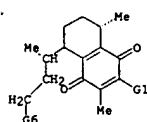
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L9 ANSWER 1 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 137:98953 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.:			US 2000-235160P	20000922

AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprise the administration of a pseudopterostatin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH<sub>2</sub>OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostatin and compds. related to pseudopterostatin are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 600 ml MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl<sub>3</sub> to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterostatin, seco-pseudopterostatin, and elisabethadiol. Pseudopterostatin had high anti-inflammatory activity.

### FIG. 1



G1 = OH  
 MPL: claim 21  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L9 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS (Continued)  
 G1 = OH  
 MPL: claim 21  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L9 ANSWER 2 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 137:15179 MARPAT  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): The Regents of the University of California, USA  
 SOURCE: PCT Int. Appl., 14 pp.  
 CODEN: PIXXO2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

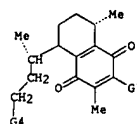
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GR, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, KZ, MD, MO, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, GQ, ML, MR, NE, SN, TD, TG

AU 2002041521 A5 20020611 AU 2002-41521 20011127  
 PRIORITY APPLN. INFO.: US 2000-253160P 20001128  
 WO 2001-US44334 20011127

AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH<sub>3</sub>, or CH<sub>2</sub>OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterostatin and compds. related to pseudopterostatin are disclosed. Examples are provided demonstrating the antiinflammatory, antiproliferative and analgesic activity of several compds. (pseudopterostatin M, seco-pseudopterostatin E, elisabethdione, etc.) isolated from P. elisabethae.

### FIG. 2



L9 ANSWER 3 OF 3 MARPAT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 110:4187 MARPAT  
 TITLE: Composition and method for rapid differentiation of  
 viable fungi from bacteria using polyene antibiotics  
 Cichanowicz, Peggy Woodruff; Belly, Robert Troconis  
 PATENT ASSIGNEE(S): Eastman Kodak Co., USA  
 SOURCE: Eur. Pat. Appl., 22 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 261931	A2	19880330	EP 1987-308380	19870922
EP 261931	A3	19891011		

R: CH, DE, FR, GB, LI  
 CA 1290226 A1 19911008 CA 1986-523203 19861118  
 PRIORITY APPLN. INFO.: US 1986-910923 19860924

AB Viable fungi are rapidly differentiated from viable bacteria by incubation with a compn. contg. a polyene antibiotic which affects membrane function in fungi and a compd. (e.g. a RIND compd. (reducible compd. which undergoes intramol. nucleophilic displacement) such as quinone I, where R1 = (R5)M(R6)Q; R2, R4 = H, (substituted) alkyl or aryl, electron-withdrawing group; R3 = R1, R2; or R3R4 complete a (substituted) strained fused carbocyclic ring; R5 = (substituted) C1-2 alkylene; R6 = (substituted) alkyl, cycloalkyl, aryl, or heterocycle; Q = C(O), C(S); X = shiftable detectable species which provides a detectable species when released; m = 0, 1) which is normally reducible by both fungi and bacteria. The antibiotic selectively inhibits the redn. of the reducible compd. by the fungi but does not affect the reducing capacity of the bacteria. A soln. contg. RIND compd. II, glucose, trimethyl-1,4-benzoquinone (electron transfer agent), buffer, and filipin (polyene antibiotic) at various dilns. was incubated with suspensions of various bacteria and fungi at 37.degree. for 30 min, and the difference in relative fluorescence before and after incubation was measured with excitation at 540 nm and emission at 620 nm. The percent inhibition of redn. of II at 0.52 mg filipin/mL was: Escherichia coli, 0; Staphylococcus aureus, 8.6; Candida albicans, 71.0; Aspergillus flavus, 42.5.

### FIG. 3

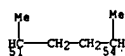
G2—G1

G1 = 6



G5 = OH  
 G7 = alkylene<(1-2)> (SO (1-) G11)  
 G4 + G6 = 51-4 54-3

L9 ANSWER 3 OF 3 MARPAT COPYRIGHT 2003 ACS (Continued)



MPL: claim 4

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(FILE 'HOME' ENTERED AT 10:46:53 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 10:47:14 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 9 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 28 MAY 2003

L4 10 S L3

FILE 'USPATFULL' ENTERED AT 10:53:47 ON 28 MAY 2003

L5 1 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 10:54:35 ON 28 MAY 2003

L7 2 S L3

L8 2 S L3 FULL

FILE 'MARPAT' ENTERED AT 10:55:51 ON 28 MAY 2003

L9 3 S L3 FULL

=> d ibib ab 1-2



## L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67994 CAPLUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:12728d-h,12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Bettolo, G. B. Marini; Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: 1st. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TETLEA; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sep'd. the CHCl<sub>3</sub> irritative fraction into 6 C<sub>15</sub>-quinones designated as mansonones A, B, C, D, E, and F, m. 117-18.degree., 68-9.degree., (C<sub>6</sub>H<sub>14</sub>), 134-8.degree., (C<sub>6</sub>H<sub>14</sub>), 173-5.degree., (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>6</sub>), 148-9.degree., (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree., (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicronron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -CH=CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C<sub>19</sub>H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicronron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b<sub>0</sub>.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, alc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formulas is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Sandermann and Dietrichs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicronron.- (H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

## L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:67993 CAPLUS  
 DOCUMENT NUMBER: 64:67993  
 ORIGINAL REFERENCE NO.: 64:12728c-d  
 TITLE: Terpenoid chemistry. XI. (-)-.beta.-Sesquiphellandrene  
 AUTHOR(S): Connell, D. W.; Sutherland, M. D.  
 CORPORATE SOURCE: Univ. Queensland, Brisbane  
 SOURCE: Australian Journal of Chemistry (1966), 19(2), 283-8  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB cf. CA 62, 5301a; 63, 14915f. A new natural sesquiterpene, (-)-.beta.-sesquiphellandrene (I), b<sub>1</sub> 90-0.5.degree., n<sub>D</sub><sup>25</sup> 1.4973, d<sub>25</sub> 0.8760, [.alpha.]<sub>D</sub><sup>25</sup> -3.99.degree. (neat), has been isolated from ginger oil in .apprx.96% purity (principal impurity (-)-.beta.-bisabolene) by distn. and gas chromatography on AgNO<sub>3</sub>-treated alumina. Rel. retentions for I on Apiezon M, butanediol succinate polyester, castor wax, and cyanosilicone (XF 1150) at 130-85.degree. are given with respect to caryophyllene, humulene, and zingiberene. On hydrogenation I yields bisabolene; reaction with anhyd. HCl in AcOH gives isozingiberene-2HCl. I nitrosite, m. 88-90.degree. (decompn.), [.alpha.]<sub>D</sub><sup>20</sup> 29.degree. (c 1.5, CHCl<sub>3</sub>), forms with NaNO<sub>2</sub>. I forms a Diels-Alder adduct with p-phenylazophenylmaleinil in the presence (but not in the absence) of (CO<sub>2</sub>H)<sub>2</sub>, m. 142.degree., [.alpha.]<sub>D</sub><sup>24</sup> -222.degree. (hexane).

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FILE 'REGISTRY' ENTERED AT 10:47:14 ON 28 MAY 2003

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 9 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 28 MAY 2003

L4 10 S L3

FILE 'USPATFULL' ENTERED AT 10:53:47 ON 28 MAY 2003

L5 1 S L3  
L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 10:54:35 ON 28 MAY 2003

L7 2 S L3  
L8 2 S L3 FULL

FILE 'MARPAT' ENTERED AT 10:55:51 ON 28 MAY 2003

L9 3 S L3 FULL

FILE 'CAOLD' ENTERED AT 10:58:13 ON 28 MAY 2003

L10 1 S L3  
SEL AN 1-

FILE 'CAPLUS' ENTERED AT 10:58:29 ON 28 MAY 2003

L11 2 S E1/OREF

=> d his

(FILE 'HOME' ENTERED AT 11:34:44 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 11:34:50 ON 28 MAY 2003

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 0 S L1 FULL

FILE 'MARPAT' ENTERED AT 11:35:47 ON 28 MAY 2003

L4 0 S L2 FULL

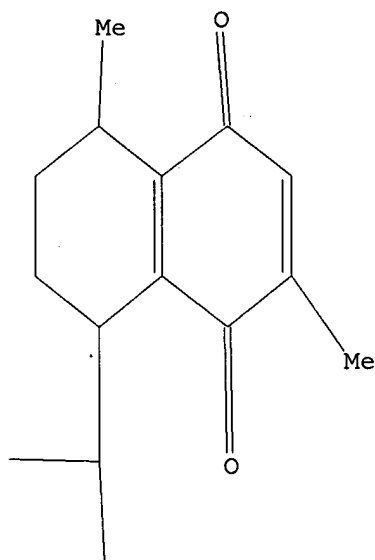
FILE 'BEILSTEIN' ENTERED AT 11:36:14 ON 28 MAY 2003

L5 0 S L1 FULL

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d ibib ab hitstr

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:685196 CAPLUS

DOCUMENT NUMBER: 123:139084

TITLE: Cadinane-type sesquiterpenes induced in *Gossypium* cotyledons by bacterial inoculation  
 AUTHOR(S): Davila-Muerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret

CORPORATE SOURCE: Dep. Biochem. Mol. Biol., Oklahoma State Univ., Stillwater, OK, 74078-0454, USA

SOURCE: Phytochemistry (1995), 39(3), 531-6

CODEN: PHYCAS; ISSN: 0031-9422

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two new sesquiterpenes, the *cis*- and *trans*-diastereomers of 7-hydroxycalamenene-2-one, as well as *trans*-7-hydroxycalamenene, were identified in exts. from cotyledons of bacterial blight-resistant *Gossypium hirsutum* harvested during the period of sesquiterpenoid phytoalexin biosynthesis following inoculation with the bacterial pathogen *Xanthomonas campestris* pv. *malvacearum*. The *cis*- and *trans*-diastereomers were distinguished by NOE correlations predicted from mol. modeling calcns.

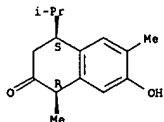
IT 155662-80-9 155662-81-0

RI: BSU (Biological study, unclassified); BIOL (Biological study) (in cotton resistant to *Xanthomonas campestris* pv. *malvacearum*)

RN 155662-80-9 CAPLUS

CN 2(1H)-Naphthalenone, 3,4-dihydro-7-hydroxy-1,6-dimethyl-4-(1-methylethyl)-, (1R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



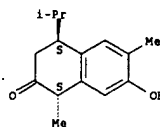
RN 155662-81-0 CAPLUS

CN 2(1H)-Naphthalenone, 3,4-dihydro-7-hydroxy-1,6-dimethyl-4-(1-methylethyl)-, (1R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

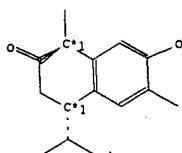
(Continued)



=> d all 16 1-2

## L6 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 7337266  
 Beilstein Pref. RN (BPR): 155662-81-0  
 CAS Reg. No. (RN): 155662-81-0  
 Chemical Name (CN): trans-7-hydroxycalamenene-2-one  
 Autonom Name (AUN): 7-hydroxy-4-isopropyl-1,6-dimethyl-3,4-dihydro-1H-naphthalen-2-one  
 Molec. Formula (MF): C15 H20 O2  
 Molecular Weight (MW): 232.32  
 Lawson Number (LN): 8807  
 File Segment (FS): racemate, Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 6257053  
 Tautomer ID (TAUTID): 6931265  
 Beilstein Citation (BSO): 6-08  
 Entry Date (DED): 1996/02/01  
 Update Date (DUPD): 1996/11/12



## Atom/Bond Notes:

1. CIP Descriptor: S

## Fragment Notes:

Additionally represents mirror image

Stereo Descriptor: +/-

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1

## L6 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

Descript	Solvent	Ref.	Note
ion			
(.KW)	(.SOL)		
Bands	CHCl3	1	1

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## Notes(s):

1. 3385 - 1618 cm<sup>-1</sup> (-1)

## UV and Visible Spectrum:

Description	Solvent	Absorption	Ext./Abs.	Ref.
(.KW)	(.SOL)	Maxima	Coeff.	
		(.AM)	(.EAC)	
		(nm)	(I/MOL*CM)	
Absorption maxima   ethanol   207.4, 284.6   21135, 3243   1				

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## Mass Spectrum:

MS

Description (.KW): spectrum

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## L6 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

ED Entry Date 1  
 UPD Update Date 1  
 CDIC Circular Dichroism 1  
 INP Isolation from Natural Product 1  
 IR Infrared Spectrum 1  
 MS Mass Spectrum 1  
 NMR Nuclear Magnetic Resonance 3  
 UVS UV and Visible Spectrum 1

## Isolation from Natural Product:

INP (INP): bacteria-inoculated cotyledons of Gossypium hirsutum

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## Circular Dichroism:

CDIC

Solvent (.SOL): ethanol  
 Note(s) (.COM): 293.2 nm

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## Nuclear Magnetic Resonance:

NMR

Description (.KW): Chemical shifts  
 Nucleus (.NUC): 1H  
 Solvents (.SOL): CDCl3  
 Temperature (.T): 8 Cel  
 Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR

Description (.KW): NOE

## Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR

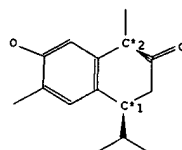
Description (.KW): Spin-spin coupling constants  
 Solvents (.SOL): CDCl3  
 Temperature (.T): 8 Cel  
 Note(s) (.COM): 1H-1H.  
 Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

## Infrared Spectrum:

## L6 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 7337265  
 Beilstein Pref. RN (BPR): 155662-80-9  
 CAS Reg. No. (RN): 155662-80-9  
 Chemical Name (CN): cis-7-hydroxycalamenene-2-one  
 Autonom Name (AUN): 7-hydroxy-4-isopropyl-1,6-dimethyl-3,4-dihydro-1H-naphthalen-2-one  
 Molec. Formula (MF): C15 H20 O2  
 Molecular Weight (MW): 232.32  
 Lawson Number (LN): 8807  
 File Segment (FS): racemate, Stereo compound  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 6257053  
 Tautomer ID (TAUTID): 6931265  
 Beilstein Citation (BSO): 6-08  
 Entry Date (DED): 1996/02/01  
 Update Date (DUPD): 1996/11/12



## Atom/Bond Notes:

1. CIP Descriptor: S

2. CIP Descriptor: R

## Fragment Notes:

Additionally represents mirror image

Stereo Descriptor: +/-

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1

L6 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

UPD Update Date 1  
INF Isolation from Natural Product 1  
MS Mass Spectrum 1  
NMR Nuclear Magnetic Resonance 6

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Isolation from Natural Product:

INP (INP): bacteria-inoculated cotyledons of  
Gossypium hirsutum

Reference(s):  
1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

Nuclear Magnetic Resonance:

NMR Description (.KW): Chemical shifts  
Nucleus (.NUC): 1H  
Solvents (.SOL): CDCl3  
Temperature (.T): 8 Cel  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR Description (.KW): Chemical shifts  
Nucleus (.NUC): 1H  
Solvents (.SOL): CDCl3  
Temperature (.T): 12 Cel  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR Description (.KW): Chemical shifts  
Nucleus (.NUC): 13C  
Solvents (.SOL): CDCl3  
Temperature (.T): 12 Cel  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR Description (.KW): NOE  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR

L6 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

Description (.KW): Spin-spin coupling constants  
Solvents (.SOL): CDCl3  
Temperature (.T): 8 Cel  
Note(s) (.COM): 1H-1H.  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

NMR

Description (.KW): Spin-spin coupling constants  
Solvents (.SOL): CDCl3  
Temperature (.T): 12 Cel  
Note(s) (.COM): 1H-1H.  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

Mass Spectrum:

MS Description (.KW): spectrum  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

Reaction:

RX

Reaction ID (.ID): 4289276  
Reactant BRN (.RBRN): 7337454  
Reactant (.RCT): 4-isopropyl-7-methoxy-1,6-dimethyl-3,4-dihydro-1H-naphthalen-2-one  
Product BRN (.PBRN): 7337265  
Product (.PRO): 7-hydroxy-4-isopropyl-1,6-dimethyl-3,4-dihydro-1H-naphthalen-2-one  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 4289276.1  
Reaction Classification (.CL): Preparation  
Reagent (.RGT): BBr3  
Reference(s):

1. Davila-Huerta, Guadalupe; Hamada, Hiroki; Davis, Gordon D.; Stipanovic, Robert D.; Adams, Christopher M.; Essenberg, Margaret, Phytochemistry, CODEN: PYTCAS, 39(3), <1995>, 531-536; BABS-5970046

=> d ibib ab hitstr 1-22 119



L19 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2003:300831 CAPLUS  
 DOCUMENT NUMBER: 138:300379  
 TITLE: Pseudopterogorgia compounds of Symbiodinium strains isolated from Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell; Mydlarz, Laura  
 PATENT ASSIGNEE(S): The Regents of the University of California, USA  
 SOURCE: PCT Int. Appl., 46 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

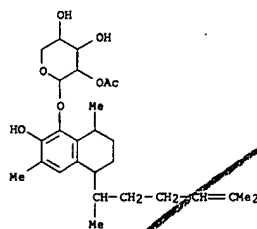
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003030820	A2	20030417	WO 2002-US31757	20021004
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				

PRIORITY APPLN. INFO.: US 2001-327028P P 20011005  
 US 2001-340833P P 20011219

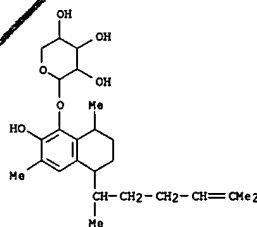
AB Disclosed herein are pseudopterogorgia compounds obtained from Symbiodinium spp. symbionts. Also disclosed are methods of obtaining, isolating, purifying or prepg. at least one pseudopterogorgia compd. comprising obtaining, isolating, purifying or prepg. the pseudopterogorgia compd. from at least one Symbiodinium spp. symbiont. In preferred embodiments, the host is Pseudopterogorgia, preferably, P. elisabethae. As disclosed, preferred pseudopterogorgia compounds and pseudopterogorgia compounds are of non-animal origin, substantially free of animal impurities, or both. Treatment methods using the pseudopterogorgia compounds and compounds are also disclosed.

IT 111397-51-4P, Seco-Pseudopterogorgia B 111466-65-0P,  
 Seco-Pseudopterogorgia A 111466-66-1P, Seco-Pseudopterogorgia C  
 111466-67-2P, Seco-Pseudopterogorgia D 433717-50-1P,  
 Seco-Pseudopterogorgia E  
 RI: NPO (Natural product occurrence); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (pseudopterogorgia compounds of Symbiodinium strains isolated from Pseudopterogorgia elisabethae)  
 RN 111397-51-4 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 2-acetate (9CI) (CA INDEX NAME)

L19 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

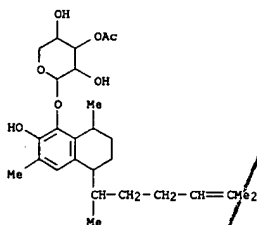


RN 111466-65-0 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)

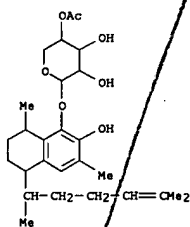


RN 111466-66-1 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate (9CI) (CA INDEX NAME)

L19 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



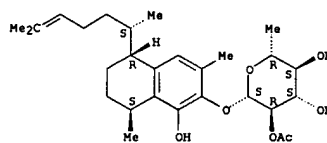
RN 111466-67-2 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate (9CI) (CA INDEX NAME)



RN 433717-50-1 CAPLUS  
 CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 2-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L19 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2002:522625 CAPLUS  
 DOCUMENT NUMBER: 137:98953  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPLN. INFO.: US 2000-235160P P 20000922				

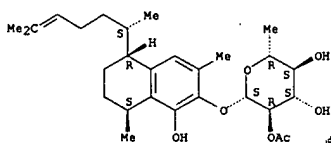
OTHER SOURCE(S): MARPAT 137:98953

AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprise the administration of a pseudopteroin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopteroin and compds. related to pseudopteroin are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 60% aq. MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopteroin, seco-pseudopteroin, and elisabethadiol. Pseudopteroin had high anti-inflammatory activity.

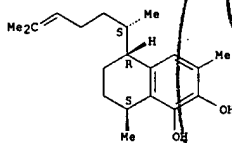
IT 433717-50-1, SecoPseudopteroin E 433717-53-4,  
 SecoPseudopteroin F 433717-55-6, SecoPseudopteroin G  
 RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)  
 (anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 433717-50-1 CAPLUS  
 CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 2-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

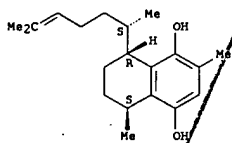


L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



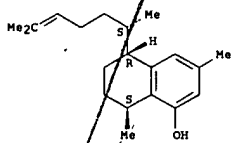
RN 433300-39-1 CAPLUS  
 CN 1,4-Naphthalenediol, 8-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2,5-dimethyl-, (5S,8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433300-41-5 CAPLUS  
 CN 1-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



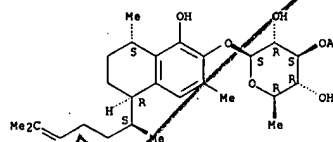
RN 433301-01-2 CAPLUS  
 CN 2-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

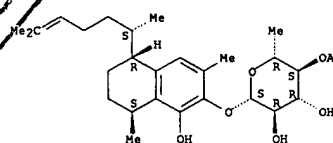
RN 433717-53-4 CAPLUS  
 CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 3-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433717-55-6 CAPLUS  
 CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 4-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

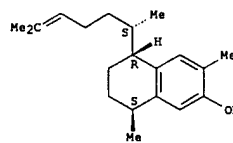


IT 199439-75-3 433300-39-1 433300-41-5,  
 Elisabethanol 433301-01-2 441019-55-2  
 441019-56-3 441019-57-4  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 199439-75-3 CAPLUS  
 CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

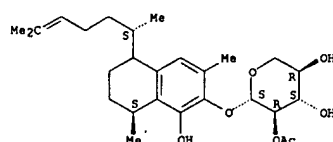
Absolute stereochemistry.

L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



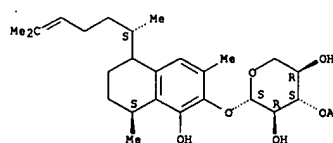
RN 441019-55-2 CAPLUS  
 CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 2-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 441019-56-3 CAPLUS  
 CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 3-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

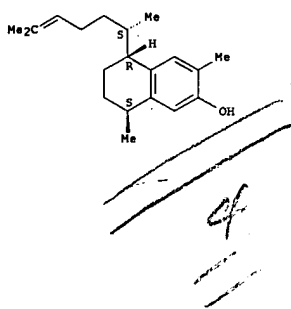


RN 441019-57-4 CAPLUS  
 CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 4-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

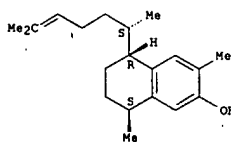


L19 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:808258 CAPLUS  
 DOCUMENT NUMBER: 134:98166  
 TITLE: Serrulatane diterpenes with antimycobacterial activity isolated from the West Indian sea whip *Pseudopterogorgia elisabethae*  
 AUTHOR(S): Rodriguez, Abimael D.; Ramirez, Catherine  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.  
 SOURCE: Journal of Natural Products (2001), 64(1), 100-102  
 CODEN: JNPADF; ISSN: 0163-3864  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Two new antimycobacterial serrulatane diterpenes, erogorgiaene (I) and 7-hydroxyerogorgiaene (II), and a novel C40 bisditerpene (V), have been isolated from the West Indian gorgonian octocoral *Pseudopterogorgia elisabethae*. The structures of compds. I-III were detd. by spectral (1D and 2D NMR, IR, UV, and HRMS) anal.  
 IT 318513-14-3P, 7-Hydroxyerogorgiaene  
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (serrulatane diterpenes with antimycobacterial activity isolated from sea whip *Pseudopterogorgia elisabethae*)  
 RN 318513-14-3 CAPLUS  
 CN 2-Naphthalenol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

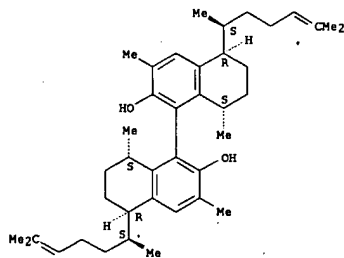
Rotation (+). Absolute stereochemistry unknown.  
 Currently available stereo shown.



IT 318513-15-4P  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (serrulatane diterpenes with antimycobacterial activity isolated from sea whip *Pseudopterogorgia elisabethae*)  
 RN 318513-15-4 CAPLUS  
 CN [1,1'-Binaphthalene]-2,2'-diol, 5,5'-bis[(1R)-1,5-dimethyl-4-hexenyl]-5,5',6,6',7,7',8,8'-octahydro-3,3',8,8'-tetramethyl-, (5S,5'S,8R,8'R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

L19 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)  
 Currently available stereo shown.



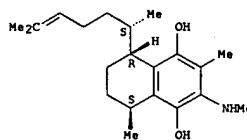
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:498626 CAPLUS  
 DOCUMENT NUMBER: 133:235399  
 TITLE: Elisabethamine: a new diterpene alkaloid from *Pseudopterogorgia elisabethae*  
 AUTHOR(S): Ata, A.; Kerr, R. G.  
 CORPORATE SOURCE: Center for Molecular Biology and Biotechnology, Department of Chemistry and Biochemistry, Florida Atlantic University, Boca Raton, FL, 33431, USA  
 SOURCE: Tetrahedron Letters (2000), 41(31), 5821-5825  
 CODEN: TETLEY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Detailed chem. studies of the methanolic ext. of *Pseudopterogorgia elisabethae*, collected from the Florida Keys, have resulted in the isolation of elisabethamine (I), a new diterpene alkaloid. Its structure was established with the aid of extensive spectroscopic studies. Compd. I exhibited cytotoxicity against lung and prostate cancer cell lines as detd. by an MTT assay.  
 IT 294202-41-8P, Elisabethamine  
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (cytotoxic diterpene alkaloid from *Pseudopterogorgia elisabethae*)  
 RN 294202-41-8 CAPLUS  
 CN 1,4-Naphthalenediol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-2-(methylamino)-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.  
 Currently available stereo shown.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:430405 CAPLUS

DOCUMENT NUMBER: 127:81637

TITLE: Chiral  $\eta^5$ -6-arene-Cr(CO)<sub>3</sub> complexes in organic synthesis: a short and highly selective synthesis of the 18-nor-seco-pseudopterosin aglycon

AUTHOR(S): Majdalani, Andre; Schmalz, Hans-Gunther

CORPORATE SOURCE: Inst. Organische Chemie, Technischen Univ., Berlin, D-10623, Germany

SOURCE: Tetrahedron Letters (1997), 38(26), 4545-4548

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:81637

AB The chiral synthetic building block 5,6-dimethoxy-1-tetralone-Cr(CO)<sub>3</sub> (I) (>99% e.e.) was converted in only nine steps and with high regio- and diastereocontrol into the 18-nor-seco-pseudopterosin aglycon II (50% overall yield). The synthesis is centrally based on the specific reactivity of the arene-Cr(CO)<sub>3</sub> substructure, esp. on the stabilization of neg. charge in benzylic position. The trans-configuration of the two benzylic substituents is secured by diastereoselective protonation of an anionic intermediate generated by conjugate addn. of 4-methyl-3-pentenyl-lithium to a complex prepd. from I via Peterson olefination, ortho-silylation and benzylic deprotonation/methylation.

IT 191791-96-5P

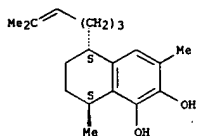
RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of 18-norsecopseudopterosin aglycon)

RN 191791-96-5 CAPLUS

CN 1,2-Naphthalenediol, 5,6,7,8-tetrahydro-3,8-dimethyl-5-(5-methyl-4-hexenyl)-, (5S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1992:486783 CAPLUS

DOCUMENT NUMBER: 117:86783

TITLE: A tricyclic diterpene from Eremophila serrulata

AUTHOR(S): Ghisalberti, E. L.

CORPORATE SOURCE: Dep. Chem., Univ. West. Australia, Nedlands, 6009, Australia

SOURCE: Phytochemistry (1992), 31(6), 2169-9

CODEN: PHYCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new tricyclic diterpene acid (I) has been isolated from Eremophila serrulata. The structure has been deduced from spectroscopic anal. and has been shown to contain the 3-epi-pseudopterosin skeleton.

IT 65003-68-1

RL: BIOL (Biological study)

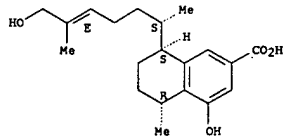
(from Eremophila serrulata)

RN 65003-68-1 CAPLUS

CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L19 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1993:124808 CAPLUS

DOCUMENT NUMBER: 118:124808

TITLE: Selective reduction of serrulatenol as a route to seco-pseudopterosin analogs

AUTHOR(S): Cowin, Linda M.; Massey-Westropp, Ralph A.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Adelaide, Adelaide, Australia

SOURCE: Journal of Natural Products (1992), 55(12), 1790-4

CODEN: JNPRDF; ISSN: 0163-3864

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Deoxygenation of serrulatenol (I; R = H) at C(13) and C(18) gave 5,8-dimethoxyserrulatenol II (R = H). Thus catalytic hydrogenation of Me ester I (R = Me) and metal/NH<sub>3</sub> cleavage of the allylic carbon-oxygen bond was followed by deoxygenation at C(18) via the Bu<sub>3</sub>Sn redn. of II (R = iodo).

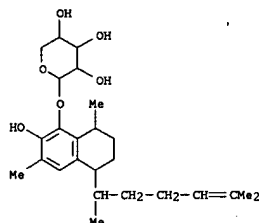
IT 145842-76-8D, analogs

RL: RCT (Reactant); RACT (Reactant or reagent)

(selective redn. of serrulatenol as a route to)

RN 145842-76-8 CAPLUS

CN 1,5-Dimethyl-4-hexenyl-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



L19 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1991:492640 CAPLUS

DOCUMENT NUMBER: 115:92640

TITLE: Controlling benzylic functionality and stereochemistry. 1. Synthesis of the secopseudopterosin aglycon

AUTHOR(S): McCombie, Stuart W.; Cox, Brian; Lin, Sue Ing; Ganguly, Ashit K.; McPhail, Andrew T.

CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA

SOURCE: Tetrahedron Letters (1991), 32(19), 2083-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:92640

AB Directed, homogeneous hydrogenation of 1-(1-hydroxymethylethyl)-5-methoxy-3,4-dihydronaphthalene (I), followed by protection and selective benzylic oxidn. gave the 1-oxo-(4R,11R) compd. II. After addn. of MeCeCl<sub>2</sub>, the natural C(1) stereochem. was established by intramol. hydride delivery from the di-t-butylsilyl ether III. Final elaboration of the sidechain and the aryl ring substituents gave the secopseudopterosin aglycon ether IV.

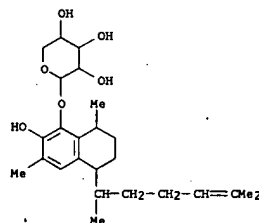
IT 111466-65-0P, Secopseudopterosin A

RL: PREP (Preparation)

(aglycon of, total synthesis of)

RN 111466-65-0 CAPLUS

CN 1.alpha.-Arabinopyranoside, [5R,8S]-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)



IT 135323-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)

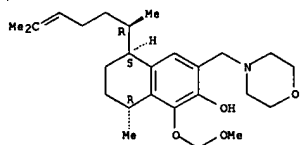
(prepn. Mannich reaction of)

RN 135323-53-4 CAPLUS

CN 2-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-1-(methoxymethoxy)-8-methyl-3-(4-morpholinylmethyl)-, [5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

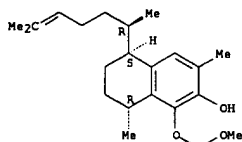
Relative stereochemistry.

L19 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



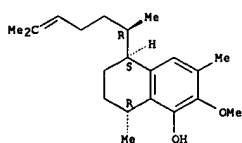
IT 135323-55-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and O-methylation of)  
 RN 135323-55-6 CAPLUS  
 CN 2-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-1-(methoxymethoxy)-3,8-dimethyl-, [5.alpha.(S\*),8.beta.] - (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 135414-41-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of)  
 RN 135414-41-4 CAPLUS  
 CN 1-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, [5.alpha.(S\*),8.beta.] - (9CI) (CA INDEX NAME)

Relative stereochemistry.



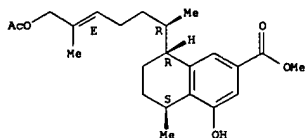
L19 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1991:471930 CAPLUS  
 DOCUMENT NUMBER: 115:71930  
 TITLE: (.eta.6-Arene)chromium complexes in organic synthesis: synthesis of (.+.-)-dihydroxysecurulic acid  
 Uemura, Motokazu; Nishimura, Hikaru; Minami, Tatsuya; Hayashi, Yuji  
 AUTHOR(S):  
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan  
 SOURCE: Journal of the American Chemical Society (1991), 113(14), 5402-10  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The title compd. I was prepd. via (.eta.6-arene)chromium complexes and involved 3 key steps: nucleophilic addn. of a dithianyl group at the meta position to an electron-donating methoxy group, trans arrangement of two benzylic substituents at C-1 and C-4 positions. and stereocontrol between C-4 and C-11 positions (exocyclic), in high regio- and stereoselectivities.

IT 130216-23-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 130216-23-8 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 8-[6-(acetyloxy)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-4-hydroxy-5-methyl-, methyl ester, [5.alpha.,8.beta.(1S\*,4E)] - (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.

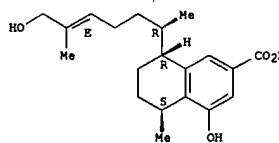


IT 130274-07-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, via arenechromium complexes)  
 RN 130274-07-6 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)] - (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.

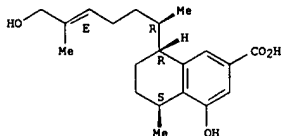
L19 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)

L19 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



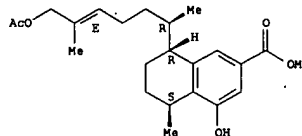
L19 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1991:82181 CAPLUS  
 DOCUMENT NUMBER: 114:82181  
 TITLE: Synthesis of (+,+-)-dihydroxysecurulic acid via  
 (arene)chromium complexes  
 AUTHOR(S): Uemura, M.; Nishimura, H.; Hayashi, Y.  
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, Japan  
 SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1990),  
 32, 403-10  
 CODEN: TYKYDS  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 AB A symposium report with 13 refs. on a highly selective synthesis of  
 (+,+-)-dihydroxysecurulic acid (I) by utilizing some characteristic  
 properties of (arene)chromium complexes.  
 IT 130274-07-6P, (+,+-)-Dihydroxysecurulic acid  
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of, via arenechromium complexes)  
 RN 130274-07-6 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-  
 1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA  
 INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



L19 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1990:612369 CAPLUS  
 DOCUMENT NUMBER: 113:212369  
 TITLE: Synthesis of (+,+-)-dihydroxysecurulic acid via  
 (arene)chromium complexes  
 AUTHOR(S): Uemura, Motokazu; Nishimura, Hikaru; Hayashi, Yuji  
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan  
 SOURCE: Tetrahedron Letters (1990), 31(16), 2319-22  
 CODEN: TETLEA; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:212369  
 AB The title compd. I was synthesized with high selectivity by utilizing some  
 characteristic properties of (arene)chromium complexes.  
 IT 130216-23-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and basic hydrolysis of)  
 RN 130216-23-8 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 8-[6-(acetyloxy)-1,5-dimethyl-4-hexenyl]-  
 5,6,7,8-tetrahydro-4-hydroxy-5-methyl-, methyl ester,  
 [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

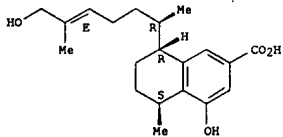
Relative stereochemistry.  
 Double bond geometry as shown.



IT 130274-07-6P, (+,+-)-Dihydroxysecurulic acid  
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (stereospecific total synthesis of)  
 RN 130274-07-6 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-  
 1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA  
 INDEX NAME)

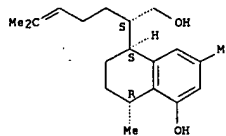
Relative stereochemistry.  
 Double bond geometry as shown.

L19 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2003 ACS (Continued)



L19 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1990:455809 CAPLUS  
 DOCUMENT NUMBER: 113:55809  
 TITLE: Diterpenes from Eremophila species  
 AUTHOR(S): Ghisalberti, Emilio L.; Jefferies, Phillip R.; Hieu  
 Thi Ngoc Vu  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands,  
 6009, Australia  
 SOURCE: Phytochemistry (1990), 29(1), 316-18  
 CODEN: PHYCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Three new diterpenes were isolated from E. macmillaniana, E. falcata, and  
 E. flaccida. In contrast to other Eremophila species, the leaf resin of  
 E. flaccida is composed of flavanones and the sesquiterpene  
 .beta.-eudesmol.  
 IT 128308-94-1  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
 BIOL (Biological study); OCCU (Occurrence)  
 (of Eremophila flaccida)  
 RN 128308-94-1 CAPLUS  
 CN 1-Naphthaleneethanol, 1,2,3,4-tetrahydro-5-hydroxy-4,7-dimethyl-.beta.-(4-  
 methyl-3-pentenyl)-, [1S-[1.alpha.(R\*),4.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



09/993,666

Page 1

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L11 ANSWER 1 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:62768 CAPLUS  
 DOCUMENT NUMBER: 136:247712  
 TITLE: Enantiospecific syntheses of pseudopterosin aglycones. Part 2. Synthesis of pseudopterosin K-L aglycone and pseudopterosin A-F aglycone via a 8.fwdarv.AB.fwdarv.BAC annulation strategy  
 AUTHOR(S): Kocienski, Philip J.; Pontiroli, Alessandro; Qun, Liu  
 CORPORATE SOURCE: Department of Chemistry, Leeds University, Leeds, LS2 9JT, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (19), 2356-2366  
 CODEN: JCSPCE; ISSN: 1472-7781  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:247712

AB The enantiomeric aglycones (I and II) of pseudopterosins K-L and A-F are synthesized from (-)- and (+)-isopulegol resp. Key features are (a) the construction of the C3 stereogenic center by a directed epoxidn.-redn. sequence (K-L); (b) the creation of the C3 stereogenic center by a Pfaltz asym. conjugate redn. (A-F); (c) benzannulation of a cyclic ketone starting with an .alpha.-oxoketene-S,S-acetal to give a tetrahydronaphthol ether; and (d) a diastereoselective intramol. electrophilic arom. substitution using an allylic sulfone as the electrophilic trigger to complete the hexahydro-1H-phenalene core. An X-ray structure of compd. III was detd.

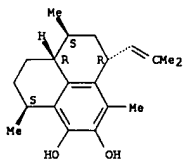
IT 106671-54-9P, Pseudopterosin A-F aglycon 404367-00-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (enantiospecific synthesis of pseudopterosin K-L aglycon and pseudopterosin A-F aglycon via annulation strategy)

RN 106671-54-9 CAPLUS

CN 1H-Phenalene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 404367-00-6 CAPLUS

CN 1H-Phenalene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3R,7S,9R,9aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L11 ANSWER 2 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:62767 CAPLUS  
 DOCUMENT NUMBER: 136:310045  
 TITLE: Enantiospecific syntheses of pseudopterosin aglycones. Part 1. Synthesis of the putative aglycone of pseudopterosin/G-J via an A.fwdarv.AB.fwdarv.ABC annulation strategy  
 AUTHOR(S): Chow, Robert; Kocienski, Philip J.; Kuhl, Alexander; LeBrazidec, Jean-Yves; Muir, Kenneth; Fish, Paul  
 CORPORATE SOURCE: Department of Chemistry, Leeds University, Leeds, LS2 9JT, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (19), 2344-2355  
 CODEN: JCSPCE; ISSN: 1472-7781  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:310045

AB The putative aglycon/I of pseudopterosin G-J and its enantiomer were synthesized enantiospecifically from 2,3-dimethoxytoluene and .eta.3-allyl cationic complexes of molybdenum and iron resp. The A.fwdarv.AB.fwdarv.ABC annulation strategy entailed the use of allyl cations or their equiv. for the creation of the three benzylic stereogenic centers. The X-ray structure of tetrahydronaphthalene II was detd.

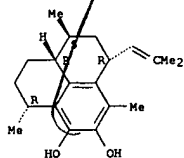
IT 406672-85-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (enantiospecific synthesis of the putative aglycon of pseudopterosin G-J via an annulation strategy)

RN 406672-85-3 CAPLUS

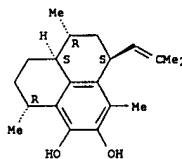
CN 1H-Phenalene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3R,7R,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 1 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:11433 CAPLUS  
 DOCUMENT NUMBER: 136:279574  
 TITLE: Total synthesis of colombiasin A and determination of its absolute configuration  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios; Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Chemistry--A European Journal (2001), 7(24), 5359-5371  
 CODEN: CEUJED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The total synthesis of the recently reported marine natural product colombiasin A (I) and detn. of its abs. configuration are reported. Two Diels-Alder cycloaddns. and a palladium-catalyzed rearrangement are employed as key reactions to construct the tetracyclic framework of the target mol. The enantioselective synthesis of colombiasin A utilizes Mikami's [(S)-BINOL-TiCl2] catalyst to asym. introduce the first chiral center during the initial Diels-Alder reaction and, in conjunction with X-ray crystallog. anal. of a bromine contg. deriv., led to the assignment of the abs. configuration of the natural product.

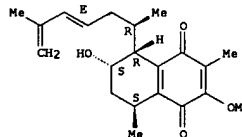
IT 362650-95-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of colombiasin A and detn. of its abs. configuration)

RN 362650-95-1 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.

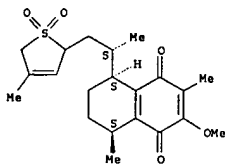


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:931849 CAPLUS  
 DOCUMENT NUMBER: 136:151319  
 TITLE: Towards colombiasin A  
 AUTHOR(S): Harrowven, David C.; Tyte, Melloney J.  
 CORPORATE SOURCE: Department of Chemistry, The University of  
 Southampton, Southampton, SO17 1BJ, UK  
 SOURCE: Tetrahedron Letters (2001), 42(49), 8709-8711  
 CODEN: TETLEY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A synthetic route to an diastereomerically unnatural analog I of  
 colombiasin A (II) is described. Key features are an arene alkylation  
 with a .gamma.-methylene-.gamma.-butyrolactone and an intramol.  
 Diels-Alder cycloaddn.  
 IT 394739-50-59  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (synthetic studies directed towards colombiasin A)  
 RN 394739-50-5 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-  
 thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-,  
 (5R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

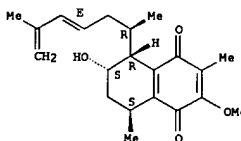


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:516801 CAPLUS  
 DOCUMENT NUMBER: 135:273093  
 TITLE: Total synthesis of Colombiasin A  
 AUTHOR(S): Nicolaou, K. C.; Vassilikogiannakis, Georgios;  
 Magerlein, Wolfgang; Kranich, Remo  
 CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for  
 Chemical Biology, The Scripps Research Institute, La  
 Jolla, CA, 92037, USA  
 SOURCE: Angewandte Chemie, International Edition (2001),  
 40(13), 2482-2486  
 CODEN: ACIEF5; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:273093

AB The authors report the total synthesis of racemic colombiasin A (I) by a  
 strategy which also delivered its C7 epimer as well as several other  
 analogs.  
 IT 362650-95-19 362651-05-69  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (total synthesis of colombiasin A)  
 RN 362650-95-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R,3E)-1,5-dimethyl-3,5-hexadienyl]-5,6,7,8-  
 tetrahydro-6-hydroxy-2-methoxy-3,8-dimethyl-, (5R,6S,8S)-rel- (9CI) (CA  
 INDEX NAME)

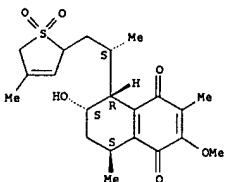
Relative stereochemistry.  
 Double bond geometry as shown.



RN 362651-05-6 CAPLUS  
 CN 1,4-Naphthalenedione, 5-[(1R)-2-(2,5-dihydro-4-methyl-1,1-dioxido-2-  
 thienyl)-1-methylethyl]-5,6,7,8-tetrahydro-6-hydroxy-2-methoxy-3,8-  
 dimethyl-, (5S,6R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L11 ANSWER 5 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

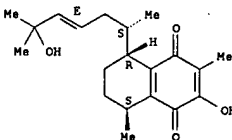
L11 ANSWER 6 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:895538 CAPLUS  
 DOCUMENT NUMBER: 134:160401  
 TITLE: Structurally diverse terpenoids from the sea whip  
 Pseudopterogorgia elisabethae (Bayer)  
 AUTHOR(S): Rodriguez, A. D.; Shi, Y.-P.  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico,  
 San Juan, 00931-3346, P. R.  
 SOURCE: Tetrahedron (2000), 56(46), 9015-9023  
 CODEN: TETRAH; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The extrn. of a specimen of Pseudopterogorgia elisabethae from Colombia  
 afforded three new diterpenes (I-III), a norditerpene (IV), and a  
 tetrasternoditerpene (V). Metabolites IV and V contain unusual carbon  
 skeletons that are previously undescribed and therefore constitute new  
 classes of C19 and C16 rearranged terpenes, resp. Full details of the  
 isolation and structure elucidation of I-V, which were established by  
 spectroscopic methods including comprehensive 2D NMR measurements, are  
 provided herein.

IT 325691-48-39  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP  
 (Properties); PUR (Purification or recovery); BIOL (Biological study);  
 OCCU (Occurrence); PREP (Preparation)  
 (terpenoids from sea whip Pseudopterogorgia elisabethae)

RN 325691-48-3 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-[(1R,3E)-5-hydroxy-  
 1,5-dimethyl-3-hexenyl]-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX  
 NAME)

Rotation (+). Absolute stereochemistry unknown.  
 Double bond geometry as shown.  
 Currently available stereo shown.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:808258 CAPLUS  
 DOCUMENT NUMBER: 134:98166  
 TITLE: Serrulatane diterpenes with antimycobacterial activity isolated from the West Indian sea whip *Pseudopterogorgia elisabethae*

AUTHOR(S): Rodriguez, Abimael D.; Ramirez, Catherine  
 CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.

SOURCE: Journal of Natural Products (2001), 64(1), 100-102  
 CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two new antimycobacterial serrulatane diterpenes, erogorgiaene (I) and 7-hydroxyerogorgiaene (II), and a novel C40 bisditerpene (V), have been isolated from the West Indian gorgonian octocoral *Pseudopterogorgia elisabethae*. The structures of compds. I-III were detd. by spectral (1D and 2D NMR, IR, UV, and HREIMS) anal.

IT 310513-14-3P, 7-Hydroxyerogorgiaene  
 RI: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

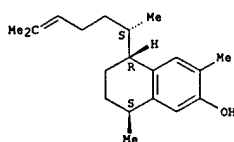
(serrulatane diterpenes with antimycobacterial activity isolated from sea whip *Pseudopterogorgia elisabethae*)

RN 310513-14-3 CAPLUS

CN 2-Naphthalenol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

Currently available stereo shown.



IT 310513-15-4P

RI: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(serrulatane diterpenes with antimycobacterial activity isolated from sea whip *Pseudopterogorgia elisabethae*)

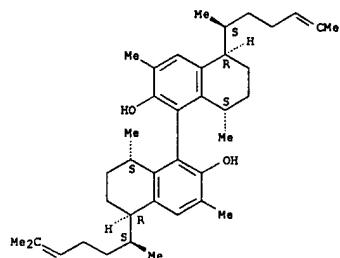
RN 310513-15-4 CAPLUS

CN [1,1'-Binaphthalene]-2,2'-diol, 5,5'-bis[(1R)-1,5-dimethyl-4-hexenyl]-5,5',6,6',7,7',8,8'-octahydro-3,3',8,8'-tetramethyl-, (5S,5'S,8R,8'R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

L11 ANSWER 7 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Currently available stereo shown.



REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:498626 CAPLUS  
 DOCUMENT NUMBER: 133:235399  
 TITLE: Elisabethamine: a new diterpene alkaloid from *Pseudopterogorgia elisabethae*

AUTHOR(S): Ata, A.; Kerr, R. G.  
 CORPORATE SOURCE: Center for Molecular Biology and Biotechnology, Department of Chemistry and Biochemistry, Florida Atlantic University, Boca Raton, FL, 33431, USA

SOURCE: Tetrahedron Letters (2000), 41(31), 5821-5825  
 CODEN: TETLEY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Detailed chem. studies of the methanolic ext. of *Pseudopterogorgia elisabethae*, collected from the Florida Keys, have resulted in the isolation of elisabethamine (I), a new diterpene alkaloid. Its structure was established with the aid of extensive spectroscopic studies. Compd. I exhibited cytotoxicity against lung and prostate cancer cell lines as detd. by an MTT assay.

IT 294202-41-8P, Elisabethamine  
 RI: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

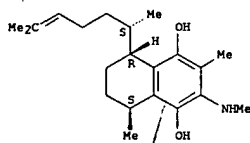
(cytotoxic diterpene alkaloid from *Pseudopterogorgia elisabethae*)

RN 294202-41-8 CAPLUS

CN 1,4-Naphthalenediol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-2-(methylamino)-, (5S,8R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

Currently available stereo shown.



REFERENCE COUNT:

11

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:442946 CAPLUS  
 DOCUMENT NUMBER: 133:208003  
 TITLE: Syntheses and Stereochemical Revision of *Pseudopterogorgia elisabethae* Aglycon and Helioporin E

AUTHOR(S): Lazewitz, Scott E.; Johnson, Ted W.; Corey, E. J.  
 CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SOURCE: Organic Letters (2000), 2(15), 2389-2392  
 CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:208003

AB Revised structures are proposed for pseudopterogorgia aglycon (I) and heliopirin E (II), based on their synthesis starting from the hexadienyltetrahydronaphthalene III.

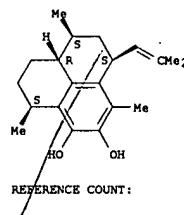
IT 290810-69-4P, Pseudopterogorgia aglycon  
 RI: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses and stereochem. revision of pseudopterogorgia aglycon and heliopirin E)

RN 290810-69-4 CAPLUS

CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7S,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

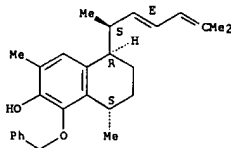


REFERENCE COUNT:

20

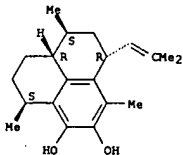
THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 34 CAPLUS COPYRIGHT 2003 ACS ON STN  
 ACCESSION NUMBER: 1998:736134 CAPLUS  
 DOCUMENT NUMBER: 130:95692  
 TITLE: A Direct and Efficient Stereocontrolled Synthetic Route to the Pseudopterrosins, Potent Marine Antiinflammatory Agents  
 AUTHOR(S): Corey, E. J.; Lazerwith, Scott E.  
 CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA  
 SOURCE: Journal of the American Chemical Society (1998), 120(49), 12777-12782  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 130:95692  
 AB Described herein is a new synthetic route to pseudopterrosin aglycon (I), a key intermediate for the synthesis of a group of antiinflammatory natural products including pseudopterrosin A and E. The pathway of synthesis starts with the abundant and inexpensive (S)-(-)-limonene and its long-known cyclic hydroboration product (II) and leads to the chiral hydroxy ketone (III). Conversion of III to (IV) followed by a novel arom. annulation produced (V) which underwent a highly diastereoselective cyclization to afford the protected pseudopterrosin aglycon (VI). The naturally occurring pseudopterrosins A and E are readily available from this key intermediate.  
 IT 219498-24-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (stereocontrolled synthesis of pseudopterrosin aglycon)  
 RN 219498-24-5 CAPLUS  
 CN 2-Naphthalenol, 5-[(1S,2E)-1,5-dimethyl-2,4-hexadienyl]-5,6,7,8-tetrahydro-3,8-dimethyl-1-(phenylmethoxy)-, (5R,8S)- (9CI) (CA INDEX NAME)  
 Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.

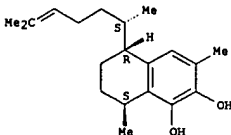


IT 106671-54-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (stereocontrolled synthesis of pseudopterrosin aglycon)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

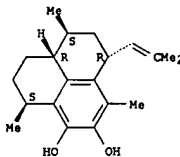
L11 ANSWER 11 OF 34 CAPLUS COPYRIGHT 2003 ACS ON STN  
 ACCESSION NUMBER: 1998:159578 CAPLUS  
 DOCUMENT NUMBER: 128:230537  
 TITLE: Preparation of heliopirin D from the seco-pseudopterrosin aglycon: revision of the stereostructure of heliopirin D  
 AUTHOR(S): Geller, Thomas; Jakupovic, Jasmin; Schmalz, Hans-Gunther  
 CORPORATE SOURCE: Institut für Organische Chemie der Technischen Universität, Berlin, D-10623, Germany  
 SOURCE: Tetrahedron Letters (1998), 39(12), 1541-1544  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A revised stereostructure for heliopirin D (I) was unequivocally established by its synthesis from the seco-pseudopterrosin aglycon and by careful anal. of NMR data. As the corresponding benzodioxole derived from the pseudopterrosin A aglycon was not identical with heliopirin E, it was proven that heliopirin D and E do not belong to the same stereochem. series.  
 IT 106671-54-9 199439-75-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. and revision of stereostructure of heliopirin D)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)  
 Absolute stereochemistry. Rotation (-).



RN 199439-75-3 CAPLUS  
 CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)  
 Absolute stereochemistry.



L11 ANSWER 10 OF 34 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)  
 Absolute stereochemistry. Rotation (-).

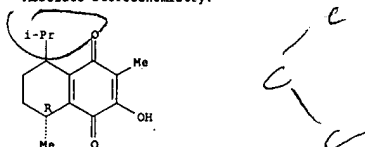


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

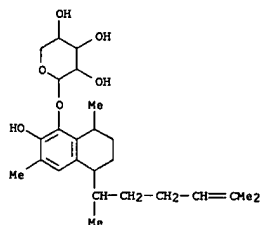
L11 ANSWER 11 OF 34 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)  
 REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:108327 CAPLUS  
 DOCUMENT NUMBER: 128:192798  
 TITLE: Formation of mansonones from naturally occurring para-benzoquinones  
 AUTHOR(S): Garcia, Esther; Mendoza, Virgilio; Agustin Guzman, J.  
 CORPORATE SOURCE: Instituto Investigaciones Químico-Biológicas, Universidad Michoacana San Nicolas de Hidalgo, Morelia, 58030, Mex.  
 SOURCE: Natural Product Letters (1997), 11(1), 67-72  
 CODEN: NPLEEF; ISSN: 1057-5634  
 PUBLISHER: Harwood Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cyclization of perezone and hydroxyperezone with HI, followed by Jones oxidn., converted them into isomansonone A and mansonone A, B, and C.  
 IT 203174-32-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of mansonones from perezone)  
 RN 203174-32-7 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



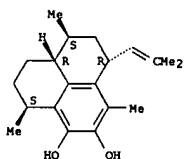
L11 ANSWER 13 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1997:749996 CAPLUS  
 DOCUMENT NUMBER: 128:34906  
 TITLE: Enantioselective synthesis of the aglycons of pseudopterodin A and seco-pseudopterodin A via a common synthetic intermediate  
 AUTHOR(S): Majdalani, Andre; Schmalz, Hans Gunther  
 CORPORATE SOURCE: Institut Organische Chemie, Technische Universität Berlin, Berlin, D-10623, Germany  
 SOURCE: Synlett (1997), (11), 1303-1305  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A synthesis proceeding in 12 steps from the chiral building block I to the key intermediate II (R = SO2Ph) from which both the title compds. are easily accessible in 2 steps is reported.  
 IT 111466-65-0P, Secopseudopterodin A  
 RL: PNU (Preparation, unclassified); PREP (Preparation) (stereoselective synthesis of pseudopterodin and seco-pseudopterodin aglycons)  
 RN 111466-65-0 CAPLUS  
 CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)



IT 106671-54-9P 199439-75-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective synthesis of pseudopterodin and seco-pseudopterodin aglycons)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

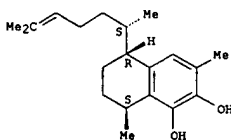
Absolute stereochemistry. Rotation (-).

L11 ANSWER 13 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



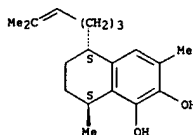
RN 199439-75-3 CAPLUS  
 CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



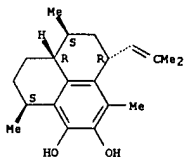
L11 ANSWER 14 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1997:430405 CAPLUS  
 DOCUMENT NUMBER: 127:81637  
 TITLE: Chiral .eta.6-arene-Cr(CO)3 complexes in organic synthesis: a short and highly selective synthesis of the 18-nor-seco-pseudopterodin aglycon  
 AUTHOR(S): Majdalani, Andre; Schmalz, Hans-Gunther  
 CORPORATE SOURCE: Inst. Organische Chemie, Technischen Univ., Berlin, D-10623, Germany  
 SOURCE: Tetrahedron Letters (1997), 38(26), 4545-4548  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 127:81637  
 AB The chiral synthetic building block 5,6-dimethoxy-1-tetralone-Cr(CO)3 (I; >99% e.e.) was converted in only nine steps and with high regio- and diastereoselectivity into the 18-nor-seco-pseudopterodin aglycon II (50% overall yield). The synthesis is centrally based on the specific reactivity of the arene-Cr(CO)3 substructure, esp. on the stabilization of neg. charge in benzylic position. The trans-configuration of the two benzylic substituents is secured by diastereoselective protonation of an anionic intermediate generated by conjugate addn. of 4-methyl-3-pentenyl-lithium to a complex prepd. from I via Peterson olefination, ortho-silylation and benzylic deprotonation/methylation.  
 IT 191791-96-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 18-norsecopseudopterodin aglycon)  
 RN 191791-96-8 CAPLUS  
 CN 1,2-Naphthalenediol, 5,6,7,8-tetrahydro-3,8-dimethyl-5-(5-methyl-4-hexenyl)-, (5S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

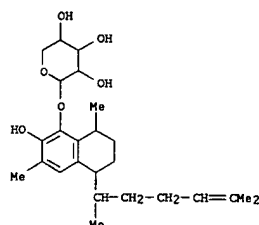


L11 ANSWER 15 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1995:1004572 CAPLUS  
 DOCUMENT NUMBER: 124:117629  
 TITLE: Total synthesis of pseudopteroin A and E aglycon  
 AUTHOR(S): Buszek, Keith R.; Bixby, Dale L.  
 CORPORATE SOURCE: Department Chemistry, Kansas State University,  
 Manhattan, KS, 66506, USA  
 SOURCE: Tetrahedron Letters (1995), 36(50), 9129-32  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 124:117629  
 AB A total synthesis of the pseudopteroin A and E aglycon I has been  
 achieved through a novel intramol. benzyne Diels-Alder cycloaddn. with a  
 substituted cyclohexadiene.  
 IT 106671-54-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of pseudopteroin A and E aglycon)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-  
 1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

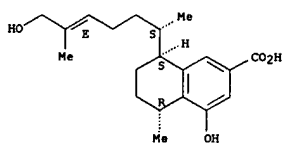


L11 ANSWER 16 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1993:124808 CAPLUS  
 DOCUMENT NUMBER: 118:124808  
 TITLE: Selective reduction of serrulatenol as a route to  
 seco-pseudopteroin analogs  
 AUTHOR(S): Cowin, Linda M.; Maszy-Westropp, Ralph A.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. Adelaide, Adelaide, Australia  
 SOURCE: Journal of Natural Products (1992), 55(12), 1790-4  
 CODEN: JNPRDF; ISSN: 0163-3864  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Deoxygenation of serrulatenol (I; R = H) at C(13) and C(18) gave  
 5,8-dimethoxyserrulatenol II (R = H). Thus catalytic hydrogenation of Me  
 ester I (R = Me) and metal/NH3 cleavage of the allylic carbon-oxygen bond  
 was followed by deoxygenation at C(18) via the Bu3Sn redn. of II (R =  
 iodo).  
 IT 145842-76-8D, analogs  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (selective redn. of serrulatenol as a route to)  
 RN 145842-76-8 CAPLUS  
 CN .beta.-D-Arabinopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-  
 2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI)  
 (CA INDEX NAME)



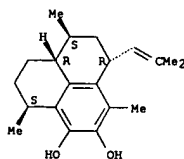
L11 ANSWER 17 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1992:486783 CAPLUS  
 DOCUMENT NUMBER: 117:86783  
 TITLE: A tricyclic diterpene from Eremophila serrulata  
 AUTHOR(S): Ghisalberti, E. L.  
 CORPORATE SOURCE: Dep. Chem., Univ. West. Australia, Nedlands, 6009,  
 Australia  
 SOURCE: Phytochemistry (1992), 31(6), 2168-9  
 CODEN: PHYCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A new tricyclic diterpene acid (I) has been isolated from Eremophila  
 serrulata. The structure has been deduced from spectroscopic anal. and  
 has been shown to contain the 3-epi-pseudopteroin skeleton.  
 IT 65003-68-1  
 RL: BIOL (Biological study)  
 (from Eremophila serrulata)  
 RN 65003-68-1 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-[6-hydroxy-  
 1,5-dimethyl-4-hexenyl]-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L11 ANSWER 18 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1991:514801 CAPLUS  
 DOCUMENT NUMBER: 115:114801  
 TITLE: Controlling benzylic functionality and  
 stereochemistry. 2. Synthesis of the pseudopteroin  
 aglycone  
 AUTHOR(S): McCombie, Stuart W.; Cox, Brian; Ganguly, Ashit K.  
 CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1991), 32(19), 2087-90  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 115:114801  
 AB Homologation, cyclization, and redn. converted the tetralin I to the  
 hexahydrophenalenol II (R=H), which was methylated to afford II (R=Me) via  
 alkoxide-directed metalation. The degree of stereoselectivity resulting  
 from reactions of II (R=Me) and congeners with allylsilane-Lewis acid  
 combinations was markedly dependent upon substitution patterns, whereas  
 Et2AlCH=SiCl4 produced pseudoaxial nitriles. The trimethylnitrile III was  
 elaborated to the pseudopteroin aglycon IV.  
 IT 135414-27-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of)  
 RN 135414-27-6 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-  
 1-propenyl)-, (3.alpha.,7.beta.,9.alpha.,9a.alpha.)- (9CI) (CA INDEX  
 NAME)

Relative stereochemistry.



L11 ANSWER 19 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:492640 CAPLUS

DOCUMENT NUMBER: 115:92640

TITLE: Controlling benzylic functionality and stereochemistry. 1. Synthesis of the secopseudopterosin aglycon

AUTHOR(S): McCombie, Stuart W.; Cox, Brian; Lin, Sue Ing; Ganguly, Ashit K.; McPhail, Andrew T.  
 CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1991), 32(19), 2083-6  
 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:92640

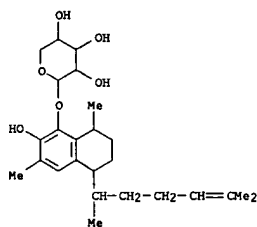
AB Directed, homogeneous hydrogenation of 1-(1-hydroxymethylethyl)-5-methoxy-3,4-dihydronaphthalene (I), followed by protection and selective benzylic oxidn. gave the 1-oxo-(4R,11R) compd. II. After addn. of MeCeCl<sub>2</sub>, the natural C(1) stereochem. was established by intramol. hydride delivery from the di-*t*-butylsilyl ether III. Final elaboration of the sidechain and the aryl ring substituents gave the secopseudopterosin aglycon ether IV.

IT 111466-65-09, Secopseudopterosin A

RL: PREP (Preparation)  
 (aglycon of, total synthesis of)

RN 111466-65-0 CAPLUS

CN .alpha.-Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)



IT 135323-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. Mannich reaction of)

RN 135323-53-4 CAPLUS

CN 2-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-1-(methoxymethoxy)-8-methyl-3-(4-morpholinylmethyl)-, [5.alpha.(S\*),8.beta.]- (9CI) (CA INDEX NAME)

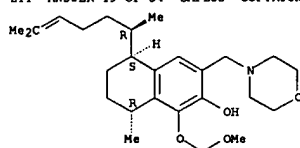
Relative stereochemistry.

L11 ANSWER 19 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

L11 ANSWER 19 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)



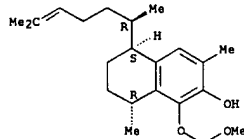
IT 135323-55-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and O-methylation of)

RN 135323-55-6 CAPLUS

CN 2-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-1-(methoxymethoxy)-3,8-dimethyl-, [5.alpha.(S\*),8.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



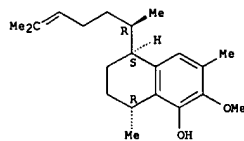
IT 135414-41-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of)

RN 135414-41-4 CAPLUS

CN 1-Naphthalenol, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-methoxy-3,8-dimethyl-, [5.alpha.(S\*),8.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:471930 CAPLUS

DOCUMENT NUMBER: 115:71930

TITLE: (.eta.6-Arene)chromium complexes in organic synthesis: synthesis of (+,+) -dihydroxysecuric acid  
 Uemura, Motokazu; Nishimura, Hikaru; Minami, Tatsuya; Hayashi, Yuji

CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan  
 SOURCE: Journal of the American Chemical Society (1991), 113(14), 5402-10

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title compd. I was prepd. via (.eta.6-arene)chromium complexes and involved 3 key steps: nucleophilic addn. of a dithianyl group at the meta position to an electron-donating methoxy group, trans arrangement of two benzylic substituents at C-1 and C-4 positions. and stereocontrol between C-4 and C-11 positions (exocyclic), in high regio- and stereoselectivities.

IT 130216-23-8P

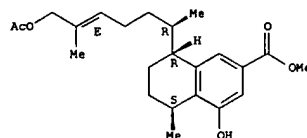
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 130216-23-8 CAPLUS

CN 2-Naphthalenecarboxylic acid, 8-[6-(acetyloxy)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-4-hydroxy-5-methyl-, methyl ester, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



IT 130274-07-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, via arenechromium complexes)

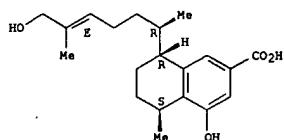
RN 130274-07-6 CAPLUS

CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

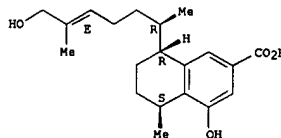
L11 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L11 ANSWER 21 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:82181 CAPLUS  
 DOCUMENT NUMBER: 114:82181  
 TITLE: Synthesis of (+-)-dihydroxyserrulatic acid via (arene)chromium complexes  
 AUTHOR(S): Uemura, M.; Nishimura, H.; Hayashi, Y.  
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, Japan  
 SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1990), 32, 403-10  
 CODEN: TYKYDS  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 AB A symposium report with 13 refs. on a highly selective synthesis of (+-)-dihydroxyserrulatic acid (I) by utilizing some characteristic properties of (arene)chromium complexes.  
 IT 130274-07-6P, (+-)-Dihydroxyserrulatic acid  
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (synthesis of, via arenechromium complexes)  
 RN 130274-07-6 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

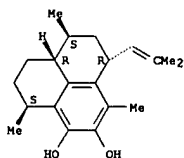
Relative stereochemistry.  
 Double bond geometry as shown.



L11 ANSWER 22 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:631727 CAPLUS  
 DOCUMENT NUMBER: 113:231727  
 TITLE: Stereospecific synthesis of the aglycone of pseudopterosin E  
 AUTHOR(S): Ganguly, A. K.; McCombie, S. W.; Cox, B.; Lin, S.; McPhail, A. T.  
 CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Pure and Applied Chemistry (1990), 62(7), 1289-91  
 CODEN: PACHAS; ISSN: 0033-4545  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A symposium contribution. Aglycon I of pseudopterosin E was synthesized from the tetralone II using several novel reactions to control stereoselectivity.  
 IT 106671-54-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from methoxytetralone)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

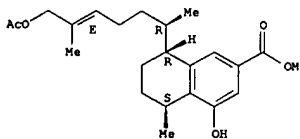
Absolute stereochemistry. Rotation (-).



L11 ANSWER 23 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

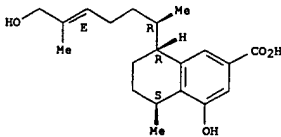
ACCESSION NUMBER: 1990:612369 CAPLUS  
 DOCUMENT NUMBER: 113:212369  
 TITLE: Synthesis of (+-)-dihydroxyserrulatic acid via (arene)chromium complexes  
 AUTHOR(S): Uemura, Motokazu; Nishimura, Hikaru; Hayashi, Yuji  
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan  
 SOURCE: Tetrahedron Letters (1990), 31(16), 2319-22  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:212369  
 AB The title compd. I was synthesized with high selectivity by utilizing some characteristic properties of (arene)chromium complexes.  
 IT 130216-23-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and basic hydrolysis of)  
 RN 130216-23-8 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 8-[6-(acetyloxy)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-4-hydroxy-5-methyl-, methyl ester, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



IT 130274-07-6P, (+-)-Dihydroxyserrulatic acid  
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (stereospecific total synthesis of)  
 RN 130274-07-6 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5.alpha.,8.beta.(1S\*,4E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.





L11 ANSWER 23 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L11 ANSWER 24 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:45809 CAPLUS  
 DOCUMENT NUMBER: 113:55809  
 TITLE: Diterpenes from Eremophila species  
 AUTHOR(S): Ghisalberti, Emilio L.; Jefferies, Phillip R.; Hieu Thi Ngoc Vu  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands, 6009, Australia  
 SOURCE: Phytochemistry (1990), 29(1), 316-18  
 CODEN: PHYTCA; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

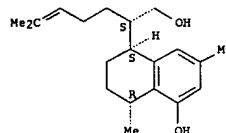
AB Three new diterpenes were isolated from *E. macmillaniana*, *E. falcata*, and *E. flaccida*. In contrast to other *Eremophila* species, the leaf resin of *E. flaccida* is composed of flavanones and the sesquiterpene .beta.-eudesmol.

IT 128308-94-1  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of *Eremophila flaccida*)

RN 128308-94-1 CAPLUS

CN 1-Naphthaleneethanol, 1,2,3,4-tetrahydro-5-hydroxy-4,7-dimethyl-.beta.-(4-methyl-3-pentenyl)-, [1S-[1.alpha.(R\*),4.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:48793 CAPLUS  
 DOCUMENT NUMBER: 112:48793  
 TITLE: Pseudopterocarins and their synthetic derivatives as anticancer, antiinflammatory and analgesic drugs  
 INVENTOR(S): Jacobs, Robert S.; Fenical, William H.  
 PATENT ASSIGNEE(S): University of California, USA  
 SOURCE: PCT Int. Appl., 45 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8901334	A1	19890223	WO 1988-US2695	19880808
V: JP				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4849410	A	19890718	US 1987-85628	19870814
CA 1317591	A1	19930511	CA 1988-574076	19880808
PRIORITY APPLN. INFO.:				
US 1987-85628 19870814				
US 1985-723214 19850415				

OTHER SOURCE(S): MARPAT 112:48793

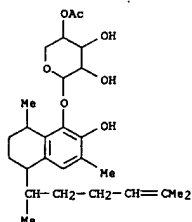
AB The title compds. I (R1-R4 = H, Cl-6 acyl; R5 = H, Me, CH2OH; R6 = Cl-10 hydroxycarbonyl) are antiinflammatory, anticancer and analgesic drugs. I (R1-R5 = H, R6 = 2-methyl-1-propenyl) (II) administered i.p. at 1-5 mg/kg, almost doubled the survival time of mice with P388 leukemia. II was extd. from *Pseudopterogorgia* with 10% MeOH in CHCl3, followed by solvent evapn., reextn. with CHCl3 and purifn. by silica gel chromatog.

IT 106665-01-4 106665-02-5 106665-03-6

RL: BIOL (Biological study)  
 (anticancer and antiinflammatory and analgesic drug)

RN 106665-01-4 CAPLUS

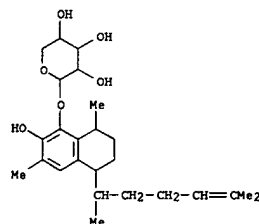
CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



RN 106665-02-5 CAPLUS

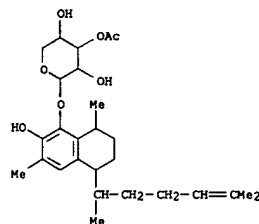
CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

L11 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 106665-03-6 CAPLUS

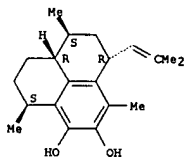
CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



L11 ANSWER 26 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1989:439720 CAPLUS  
 DOCUMENT NUMBER: 111:39720  
 TITLE: Enantiospecific total synthesis of pseudopterins A and E  
 AUTHOR(S): Corey, E. J.; Carpino, Philip  
 CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA  
 SOURCE: Journal of the American Chemical Society (1989), 111(14), 5472-4  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 111:39720

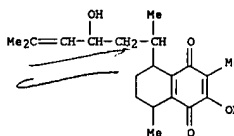
AB A total, enantiospecific synthesis of pseudopterins A (I) and E (II) has been achieved starting from (+)-menthol via the known hydroxy oxime III. The chiral octalone IV, synthesized from III, was transformed into the tricyclic keto phenol V using a novel arom. annulation process involving 2 intermediates. V was ortho hydroxylated to the catechol deriv. which, after protection as the isopropylidene deriv., was elaborated to the pseudopterin aglycon. A novel and effective  $\alpha$ -L-fucosylation of the aglycon gave II. The aglycon was also converted selectively to the tosylate and thence to I using 2,3,4-triacetyl- $\alpha$ -D-xylopyranosyl bromide.  
 IT 106671-54-9P  
 RI: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, intermediate in total synthesis of pseudopterins A and E)  
 RN 106671-54-9 CAPLUS  
 CN 1H-Phenylene-4,5-diol, 2,3,7,8,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

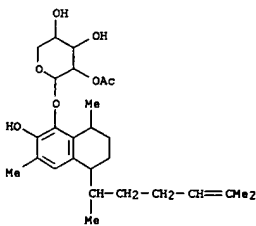


L11 ANSWER 27 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1989:21335 CAPLUS  
 DOCUMENT NUMBER: 110:21335  
 TITLE: New marine diterpenoids, including a unique hydroperoxide, from a Caribbean gorgonian coral of the genus Pseudopterogorgia  
 AUTHOR(S): Harvis, Carl A.; Burch, Mark T.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Scripps Inst. Oceanogr., La Jolla, CA, 92093-0228, USA  
 SOURCE: Tetrahedron Letters (1988), 29(35), 4361-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 110:21335

AB 4 New diterpenoids (I-IV) related to the aglycon components of the recently described pseudopterins and seco-pseudopterins have been isolated from an undescribed Pseudopterogorgia species from the Caribbean Sea. The new compds., described on the basis of their NMR properties and chem. interconversions, appear to be related, illustrating some interesting rearrangements of a tertiary hydroperoxide in this series.  
 IT 118169-36-1  
 RI: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (of gorgonian coral)  
 RN 118169-36-1 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-5-(3-hydroxy-1,5-dimethyl-4-hexenyl)-3,8-dimethyl- (9CI) (CA INDEX NAME)

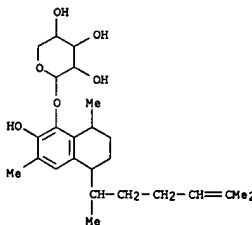


L11 ANSWER 28 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1987:633406 CAPLUS  
 DOCUMENT NUMBER: 107:233406  
 TITLE: The seco-pseudopterins, new anti-inflammatory diterpene-glycosides from a Caribbean gorgonian octocoral of the genus Pseudopterogorgia  
 AUTHOR(S): Look, Sally A.; Fenical, William  
 CORPORATE SOURCE: Inst. Mar. Resour., Univ. California, San Diego, La Jolla, CA, 92093, USA  
 SOURCE: Tetrahedron (1987), 43(15), 3363-70  
 CODEN: TETRAH; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A new class of diterpene-pentosides, the seco-pseudopterins A-D (I, II, III, and IV) were isolated from a Caribbean sea whip of the genus Pseudopterogorgia. The new compds. are arabinose glycosides possessing aglycons of the serrulatane class, the compds. in the series are monosaccharide positional isomers, and they are related to the recently described pseudopterins by bond cleavage at the C5 - C13 positions. The seco-pseudopterins possess potent anti-inflammatory and analgesic activities equiv. to com. anti-inflammatory drugs. The structures of these new compds. are suggested on the basis of comprehensive spectral analyses and chem. transformations.  
 IT 111397-51-4 111466-65-0 111466-66-1  
 RI: BIOL (Biological study)  
 (of gorgonian octocoral, isolation and mol. structure and anti-inflammatory activity of)  
 RN 111397-51-4 CAPLUS  
 CN  $\alpha$ -Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 2-acetate (9CI) (CA INDEX NAME)

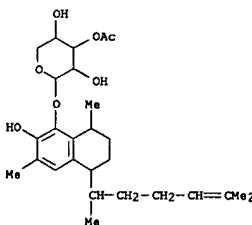


RN 111466-65-0 CAPLUS  
 CN  $\alpha$ -Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl (9CI) (CA INDEX NAME)

L11 ANSWER 28 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 111466-66-1 CAPLUS  
 CN  $\alpha$ -Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate (9CI) (CA INDEX NAME)

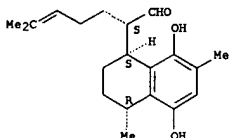


RN 111466-67-2 CAPLUS  
 CN  $\alpha$ -Arabinopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate (9CI) (CA INDEX NAME)



L11 ANSWER 30 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1985:611133 CAPLUS  
 DOCUMENT NUMBER: 103:211133  
 TITLE: Eremophilane and serrulatane terpenoids from Eremophila rotundifolia  
 AUTHOR(S): Abell, Andrew D.; Massey-Westropp, Ralph A.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. Adelaide, Adelaide, 5001, Australia  
 SOURCE: Australian Journal of Chemistry (1985), 38(8), 1263-9  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The new terpenoids 9-oxoeremophila-10,11(13)-dien-12-al (I) and 5,8-dihydroxyserrulat-14-en-18-al (II) were isolated from E. rotundifolia. Their abs. stereochem. was established by chem. correlation with known compds.  
 IT 99305-32-5  
 RL: BIOL (Biological study)  
 (from Eremophila rotundifolia, structure of)  
 RN 99305-32-5 CAPLUS  
 CN 1-Naphthaleneacetaldehyde, 1,2,3,4-tetrahydro-5,8-dihydroxy-4,7-dimethyl- $\alpha$ -(4-methyl-3-pentenyl)-, [1S-[1.alpha.(R\*),4.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

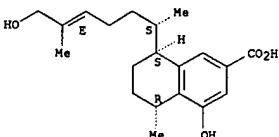


IT 99305-21-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of)  
 RN 99305-21-2 CAPLUS  
 CN 1,4-Naphthalenediol, 5,6,7,8-tetrahydro-8-[(1-hydroxymethyl)-5-methyl-4-hexenyl]-2,5-dimethyl-, [5R-[5.alpha.,8.beta.(5\*)]]- (9CI) (CA INDEX NAME)

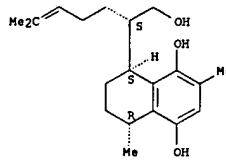
Absolute stereochemistry.

L11 ANSWER 31 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1980:146967 CAPLUS  
 DOCUMENT NUMBER: 92:146967  
 TITLE: The chemistry of Eremophila spp. XI. The absolute configuration of dihydroxyserrulatic acid  
 AUTHOR(S): Croft, Kevin D.; Ghisalberti, Emilio L.; Jefferies, Phillip R.; Stuart, Alan D.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands, 6009, Australia  
 SOURCE: Australian Journal of Chemistry (1979), 32(9), 2079-83  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The (1'S)-configuration of dihydroxyserrulatic acid (I), isolated from E. serrulata, was detd. by transformation into the (1'S)-dimethylhexylnaphthalene II and by synthesis of its enantiomer III from (R)-citronellal.  
 IT 65003-68-1  
 RL: PRP (Properties)  
 (abs. configuration of)  
 RN 65003-68-1 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

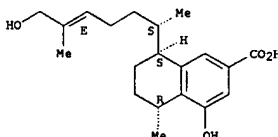


L11 ANSWER 30 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L11 ANSWER 32 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1978:7095 CAPLUS  
 DOCUMENT NUMBER: 88:7095  
 TITLE: The chemistry of Eremophila spp. VI. Stereochemistry and crystal structure of dihydroxyserrulatic acid  
 AUTHOR(S): Croft, Kevin D.; Ghisalberti, Emilio L.; Jefferies, Phillip R.; Raston, Colin L.; White, Allan H.; Hall, Sydney R.  
 CORPORATE SOURCE: Crystallogr. Cent., Univ. West. Australia, Nedlands, Australia  
 SOURCE: Tetrahedron (1977), 33(12), 1475-80  
 CODEN: TETRAH; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The structure of the title compd. (I) (from E. serrulata), a diterpenoid analog of codinene, was detd. I was characterized by chem. and spectral data and its relative stereochem. established by x-ray diffraction at 295 K. Std. dehydrn. of I gave the naphthalene II.  
 IT 65003-68-1P  
 RL: PREP (Preparation)  
 (from Eremophila serrulata, structure detn. of)  
 RN 65003-68-1 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, [5R-[5.alpha.,8.beta.(1S\*,4E)]]- (9CI) (CA INDEX NAME)

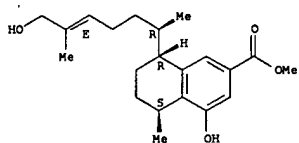
Absolute stereochemistry.  
 Double bond geometry as shown.



IT 65003-60-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and acetylation of)  
 RN 65003-60-3 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-4-hydroxy-8-(6-hydroxy-1,5-dimethyl-4-hexenyl)-5-methyl-, methyl ester, [5.alpha.,8.beta.(1S\*,4E)]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.  
 Double bond geometry as shown.

L11 ANSWER 32 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



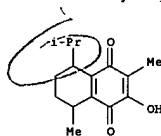
L11 ANSWER 33 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1967:105061 CAPLUS  
 DOCUMENT NUMBER: 66:105061  
 TITLE: Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Marini-Bettolo, Giovanni B.; Casinovi, Carlo G.; Galeffi, Corrado; Delle Monache, Franco; Del Guercio, G.  
 CORPORATE SOURCE: Univ. Cattolica, Rome, Italy  
 SOURCE: Annali dell'Istituto Superiore di Sanita (1966), 2(2-3), 327-41  
 CODEN: AISSAW; ISSN: 0021-2571  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Italian

AB CA 64, 12728d. The wood of *M. altissima*, which is widely used for furniture making, was studied for the irritating and cardiokinetic substances it contains. By means of column chromatog., the crude CHCl<sub>3</sub> ext. of *M. altissima* was fractionated into 6 new quinones: red mansonone A (I), m. 117-18.degree., (.alpha.)20D 680.degree. (c 0.2, CHCl<sub>3</sub>); gold-yellow mansonone B (II), 68-9.degree.; orange mansonone C (III), m. 134-8.degree.; orange mansonone D (IV), m. 173-5.degree.; orange-yellow mansonone E (V), m. 148-9.degree.; violet-mansonone F (VI), m. 214-15.degree.. Their structures were partially elucidated by chem. and spectroscopic analysis. A C15 skeleton which is a common feature for the compds. suggests a terpene origin. Two have the structure of oxaphenylene found the 1st time in biflorin. I was easily reduced in H<sub>2</sub>O with Na hydrosulfite. I was reduced with Zn in Ac<sub>2</sub>O and pyridine to yield the diacetate, m. 158-60.degree.. Ac<sub>2</sub>O and NaOAc yielded the acetate, b0.02 120.degree.. II, III, IV, and V were reduced by Na hydrosulfite and reoxidized by air. III with pyridine, Ac<sub>2</sub>O, and Zn yielded the diacetate, m. 156-8.degree.. Boiling with an acetic acid soln. of o-phenylenediamine yielded the quinoxaline, m. 103-4.degree.. IV did not react with Ac<sub>2</sub>O and NaOAc. With Zn and Ac<sub>2</sub>O and pyridine it gave a diacetyl deriv. With o-phenylenediamine and acetate V gave a deriv., m. 148-50.degree.. With Zn, Ac<sub>2</sub>O, and pyridine V gave a diacetate, m. 110.degree.. VI is very sensitive to light and changes with time, especially in soln.

IT 14375-53-2  
 RL: FRP (Properties)  
 (structure of)

RN 14375-53-2 CAPLUS  
 CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



L11 ANSWER 34 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1966:67994 CAPLUS  
 DOCUMENT NUMBER: 64:67994  
 ORIGINAL REFERENCE NO.: 64:12728d-h, 12729a  
 TITLE: New class of quinones. Sesquiterpenoid quinones of *Mansonia altissima*  
 AUTHOR(S): Bettolo, G. B.; Marini, Casinovi, C. G.; Galeffi, C.  
 CORPORATE SOURCE: 1st. Super. Sanita, Rome  
 SOURCE: Tetrahedron Letters (1965), (52), 4857-64  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

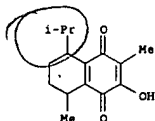
AB To sep. the irritative from the cardiac principles, the heartwood of *M. altissima* was submitted to systematic solvent extn. in which the 2 main pharmacol.-active principles appeared in the CHCl<sub>3</sub> and EtOH exts., resp. Column chromatography on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from an adequate series of solvents (C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub>, AcOEt) sepd. the CHCl<sub>3</sub> irritative fraction into 6 C15-quinones designated as mansonones A, B, C, D, E, and F, m. 117-18.degree. (C<sub>6</sub>H<sub>12</sub>), 68-9.degree. (C<sub>6</sub>H<sub>14</sub>), 134-8.degree. (C<sub>6</sub>H<sub>14</sub>), 173-5.degree. (C<sub>6</sub>H<sub>12</sub>C<sub>6</sub>H<sub>6</sub>), 148-9.degree. (C<sub>6</sub>H<sub>12</sub>), and 214-15.degree. (C<sub>6</sub>H<sub>6</sub>), resp. Mansonone F, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, characterized by its deep violet color, was reactive to .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub>, inert to acetylation and lacked OH absorption in the ir spectrum (N.M.R. spectrum given). The presence of a tricyclic 1,2-naphthoquinone (I) with the fragment -CMe:CHO-, in the 3rd ring, similar in structure to dihydrobiflorin was suggested. Mansonone E (II) on reductive acetylation gave a diacetate, C<sub>19</sub>H<sub>20</sub>O<sub>5</sub>, m. 110.degree.. II reacted with .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give the expected quinoxaline, m. 148-50.degree.. The ir spectra of II was similar to that of tetrahydrobiflorin. Mansonone C (III), gave a quinoxaline deriv., m. 103-4.degree., and was converted by reductive acetylation to a diacetate, m. 156-8.degree.. On the assumption of a common biogenesis with I and II it was deduced that III was identical with the cadalene 7,8-quinone of Lindahl (CA 49, 8223g). Mansonone B (IV) (monoacetate b0.02 120.degree.) .lambda. 263,339, 435 m.mu. (log .epsilon. 4.1, 2.53, 1.8, slc.) may have one of the 2 alternative formulas given. Mansonone A (V) showed absence of aromatic protons and benzylic methylenes and the proposed formulas is in accordance with those of I-IV and with the isoprene rule. V is probably identical with the compd. described by Sandermann and Dietrichs (CA 53, 14351e). Mansonone D (VI) gave no acetate but reacted with .omicron.-(H<sub>2</sub>N)2C<sub>6</sub>H<sub>4</sub> to give a quinoxaline. A tentative structure was assigned. Spectral data were given for the compds.

IT 14375-53-2, Mansonone B

(structure of)

RN 14375-53-2 CAPLUS

CN 1,4-Naphthalenedione, 5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



=> d ibib ab hitstr 1-3

L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2002522625 CAPLUS  
 DOCUMENT NUMBER: 137:98953  
 TITLE: Anti-inflammatory compounds derived from  
 Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127

PRIORITY APPLN. INFO.: US 2000-235160P P 20000922

OTHER SOURCE(S): MARPAT 137:98953

AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprise the administration of a pseudopterostin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an Cl-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 60% aq. MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterostins, seco-pseudopterostins, and elisabethadiol. Pseudopterostins had high anti-inflammatory activity.

IT 433717-50-1, SecoPseudopterostin E 433717-53-4,  
 SecoPseudopterostin F 433717-55-6, SecoPseudopterostin G  
 433717-71-6, Elisabethadione  
 RI: NPO (Natural product occurrence); PAC (Pharmacological activity); THU  
 (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES  
 (Uses)

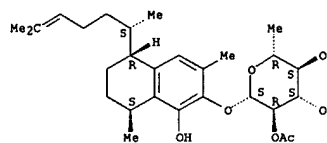
(anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 433717-50-1 CAPLUS

CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 2-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

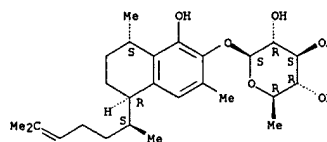
L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 433717-53-4 CAPLUS

CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 3-acetate (9CI) (CA INDEX NAME)

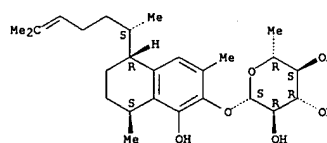
Absolute stereochemistry.



RN 433717-55-6 CAPLUS

CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 4-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

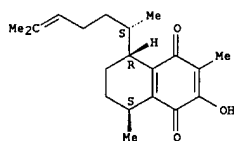


RN 433717-71-6 CAPLUS

CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 199439-75-3 433300-39-1 433300-41-5,

Elisabethanol 433331-01-2 441019-54-1

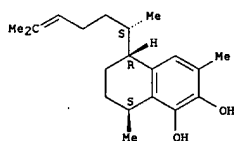
441019-55-2 441019-56-3 441019-57-4

RI: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (anti-inflammatory compds. from Pseudopterogorgia elisabethae)

RN 199439-75-3 CAPLUS

CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

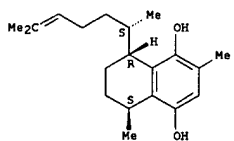
Absolute stereochemistry.



RN 433300-39-1 CAPLUS

CN 1,4-Naphthalenediol, 8-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2,5-dimethyl-, (5S,8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

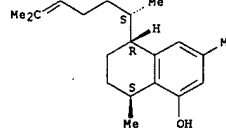


RN 433300-41-5 CAPLUS

CN 1-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

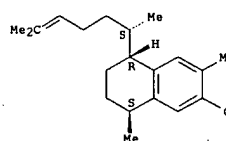
L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 433331-01-2 CAPLUS

CN 2-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

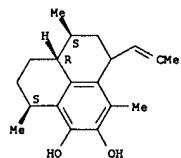
Absolute stereochemistry.



RN 441019-54-1 CAPLUS

CN 1H-Phenylene-4,5-diol, 2,3,7,8,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

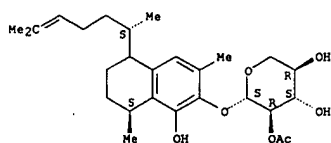


RN 441019-55-2 CAPLUS

CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 2-acetate (9CI) (CA INDEX NAME)

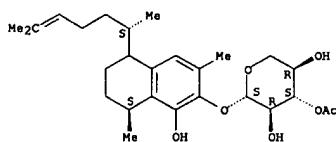
Absolute stereochemistry.

L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



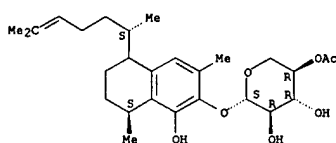
RN 441019-56-3 CAPLUS  
CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 3-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



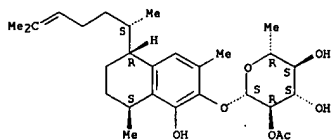
RN 441019-57-4 CAPLUS  
CN .beta.-D-Xylopyranoside, (8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl, 4-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



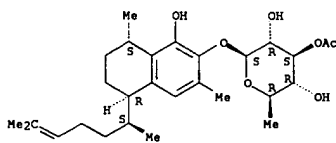
L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)  
tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 2-acetate (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



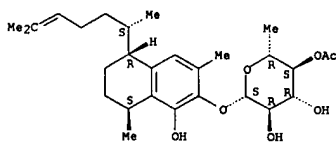
RN 433717-53-4 CAPLUS  
CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 3-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433717-55-6 CAPLUS  
CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-1-hydroxy-3,8-dimethyl-2-naphthalenyl 6-deoxy-, 4-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433717-71-6 CAPLUS  
CN 1,4-Naphthalenedione, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2002:428919 CAPLUS  
DOCUMENT NUMBER: 137:15779  
TITLE: Anti-inflammatory compounds derived from Pseudopterogorgia elisabethae  
INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
PATENT ASSIGNEE(S): The Regents of the University California, USA  
SOURCE: PCT Int. Appl., 44 pp.  
CODEN: PIXX02  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

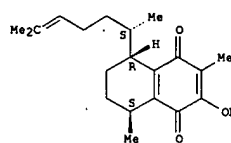
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002/044191	A2	20020606	WO 2001-US44334	20011127
WO 2002/044191	A3	20030417		

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GM, GH, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002/041521 A5 20020611 AU 2002-41521 20011127  
EP 1339729 A2 20030903 EP 2001-988191 20011127  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
PRIORITY APPLN. INFO.: US 2000-253160 P 20001128  
WO 2001-US44334 W 20011127

OTHER SOURCE(S): MARPAT 137:15779  
AB Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterins and compds. related to pseudopterins are disclosed. Examples are provided demonstrating the antiinflammatory, antiproliferative and analgesic activity of several compds. (pseudopterins M, seco-pseudopterins E, elisabethdione, etc.) isolated from P. elisabethae.  
IT 433717-50-1P, Secopseudopterin E 433717-53-4P, Secopseudopterin F 433717-55-6P, Secopseudopterin G 433717-71-6P, Elisabethdione  
RI: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(pharmacol. activity of compds. derived from Pseudopterogorgia elisabethae)  
RN 433717-50-1 CAPLUS  
CN .beta.-D-Glucopyranoside, (5R,8S)-5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-

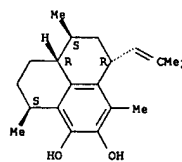
L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 106671-54-9 199439-75-3 433300-39-1  
433300-41-5 433331-01-2  
RI: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pharmacol. activity of compds. derived from Pseudopterogorgia elisabethae)

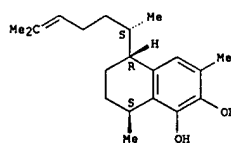
RN 106671-54-9 CAPLUS  
CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, (3S,7R,9S,9aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 199439-75-3 CAPLUS  
CN 1,2-Naphthalenediol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

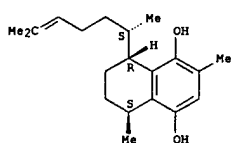


RN 433300-39-1 CAPLUS  
CN 1,4-Naphthalenediol, 8-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-2,5-dimethyl-, (5S,8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

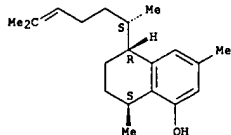


L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



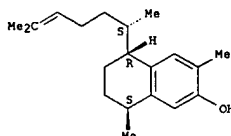
RN 433300-41-5 CAPLUS  
CN 1-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433331-01-2 CAPLUS  
CN 2-Naphthalenol, 5-[(1S)-1,5-dimethyl-4-hexenyl]-5,6,7,8-tetrahydro-3,8-dimethyl-, (5R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:84986 CAPLUS  
DOCUMENT NUMBER: 106:84986  
TITLE: Pseudopterisin and its synthetic derivatives  
INVENTOR(S): Jacobs, Robert S.; Fenical, William H.  
PATENT ASSIGNEE(S): University of California, Berkeley, USA  
SOURCE: Eur. Pat. Appl., 31 pp.  
CODEN: EPXKXW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 198689	A2	19861022	EP 1986-302711	19860411
EP 198689	A3	19870610		
R:	AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE			
US 4745104	A	19880517	US 1985-723214	19850415
CA 1288771	A1	19910910	CA 1986-505110	19860326
ZA 8602488	A	19861126	ZA 1986-2488	19860403
DK 8601626	A	19861016	DK 1986-1626	19860410
AU 8656065	A1	19861023	AU 1986-56065	19860414
ES 553952	A1	19871101	ES 1986-553952	19860414
JP 62036395	A2	19870217	JP 1986-85238	19860415
JP 2748001	B2	19980506		

PRIORITY APPLN. INFO.: US 1985-723214 19850415

AB The title compds. I [R1-R4 = H, C1-6 acyl; R5 = H, HOCH<sub>2</sub>; R6 = (un)substituted hydrocarbonyl] were isolated from Caribbean gorgonians or prepd. and tested for analgesic and antiinflammatory activity. Thus, pseudopterisin A (R1-R5 = H, R6 = Me<sub>2</sub>C:CH) was acetylated with Ac<sub>2</sub>O in pyridine to give 79% I (R1-R4 = Ac, R5 = H, R6 = Me<sub>2</sub>C:CH) (II). In the phenylquinone writhing test in mice 25 mg II/kg s.c. reduced writhing 34%.

IT 106665-01-4 106665-02-5 106665-03-6  
106671-55-0

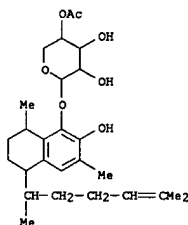
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USEB (Use)

[analgesic and antiinflammatory activity of]

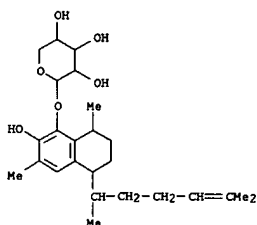
RN 106665-01-4 CAPLUS

CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 4-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

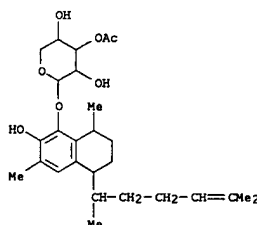


RN 106665-02-5 CAPLUS  
CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)



RN 106665-03-6 CAPLUS  
CN .beta.-D-Xylopyranoside, 5-(1,5-dimethyl-4-hexenyl)-5,6,7,8-tetrahydro-2-hydroxy-3,8-dimethyl-1-naphthalenyl, 3-acetate, [5R-[5.alpha.(S\*),8.beta.]]- (9CI) (CA INDEX NAME)

L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 106671-55-0 CAPLUS

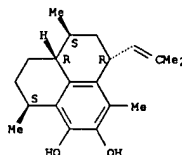
CN 1H-Phenylene-4,5-diol, 2,3,7,8,9,9a-hexahydro-3,6,9-trimethyl-7-(2-methyl-1-propenyl)-, monoacetate, [3S-(3.alpha.,7.beta.,9.alpha.,9a.alpha.]]- (9CI) (CA INDEX NAME)

CH 1

CRN 106671-54-9

CMF C20 H28 O2

Absolute stereochemistry. Rotation (-).



CH 2

CRN 64-19-7

CMF C2 H4 O2



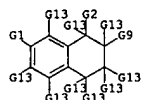
=> d ibib ab fqhit 1-21

L19 ANSWER 1 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 139:159969 MARPAT  
 TITLE: Nonsteroidal analogs of 2-methoxyestradiol for treatment of diseases characterized by undesirable angiogenesis and proliferative activity  
 INVENTOR(S): Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Treaston, Anthony M.; Pribluda, Victor S.  
 PATENT ASSIGNEE(S): Entremed, Inc., USA  
 SOURCE: PCT Int. Appl., 49 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003063791	A2	20030807	WO 2003-US2917	20030130
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

US 2003187076 A1 20031002 US 2003-354921 20030130  
 PRIORITY APPL. INFO.: US 2002-354046P 20020130  
 AB The invention provides compns. and methods for treating mammalian disease characterized by undesirable angiogenesis and proliferative activity by administering nonsteroidal deriva. of 2-methoxyestradiol, e.g. I (prepn. described).

MSTR 1



G2 = Me  
 G13 = alkenyl (SO) / 137 / OH (SO)

137(0)G4

MPL: claim 1

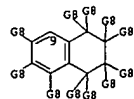
L19 ANSWER 2 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 138:238176 MARPAT  
 TITLE: Preparation of amides as Rho kinase inhibitors  
 INVENTOR(S): Uehata, Masayoshi; Takanashi, Shinichi; Hamaguchi, Seiji  
 PATENT ASSIGNEE(S): Mitsubishi Pharma Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 68 pp.  
 CODEN: JI00XAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003073357	A2	20030312	JP 2001-266055	20010903
PRIORITY APPL. INFO.: JP 2001-266055 20010903 AB The title amides RaN(Rb)CORc [Ra = (un)substituted N-contg. heterocyclic ring; Rb = H, etc.; Rc = aryl, etc.] are prepd. Comps. of this invention in vitro showed IC50 values of 23 nM to 48 nM against human Rho kinase. Formulations are given.				

MSTR 1

G1—G4—C(O)—G6

G6 = 9



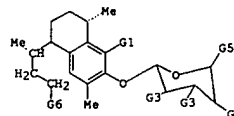
G8 = alkyl<(1-18)> (SO (1- G3) / CN / OH / acyl  
 DER: or pharmaceutically acceptable salts or hydrates  
 MPL: claim 1

L19 ANSWER 1 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

L19 ANSWER 3 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 137:98953 MARPAT  
 TITLE: Anti-inflammatory compounds derived from Pseudopterogorgia elisabethae  
 INVENTOR(S): Jacobs, Robert S.; Kerr, Russell G.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 20 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091093	A1	20020711	US 2001-993666	20011127
PRIORITY APPL. INFO.: US 2000-235160P 20000922 AB Methods for treating, preventing, or inhibiting diseases and disorders assocd. with inflammation, cell-proliferation, and pain comprise the administration of a pseudopterostin (I, R1 = e.g., H, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having 2-20 carbon atoms, R2, R3, and R4 = each independently H or an C1-6 acyl, R5 = H, Me, or CH2OH, and R6 = hydrocarbon with 1-10 carbon atoms) are disclosed. Other seco-pseudopterostins and compds. related to pseudopterostins are disclosed. About 1.0 kg P. elisabethae was freeze-dried and extd. with MeOH and followed with 2 chloroform extns. The solvent was evapd. under reduced pressure to give 360 g a gum. This gum was then re-dissolved in 600 ml MeOH which was partitioned with hexane to give 202 g hexane ext. This defatted ext. was then extd. with CHCl3 to yield 11.5 g an oil which chromatographed on a silica gel column to give various pseudopterostins, seco-pseudopterostins, and elisabethadiol. Pseudopterostins had high anti-inflammatory activity.				

MSTR 2



G1 = OH  
 G6 = hydrocarbyl<(1-10)>  
 MPL: claim 11  
 NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L19 ANSWER 4 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

137:15779 MARPAT

TITLE:

Anti-inflammatory compounds derived from

Pseudopterosorgia elisabethae

INVENTOR(S):

Jacobs, Robert S.; Kerr, Russell G.

PATENT ASSIGNEE(S):

The Regents of the University California, USA

SOURCE:

PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044191	A2	20020606	WO 2001-US44334	20011127
WO 2002044191	A3	20030417		
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, T2, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002041521	A5	20020611	AU 2002-41521	20011127
EP 1339729	A2	20030903	EP 2001-988191	20011127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:

US 2000-253160P 20001128

WO 2001-US44334 20011127

AB

Methods for treating, preventing, or inhibiting diseases and disorders associated with inflammation, cell-proliferation, and pain comprising the administration of a compd. having the structural formula I wherein R1 is a hydrogen, alkyl, aryl, hydroxyalkyl, cycloalkyl, cycloalkenyl, carboxylic acid, alkylamino or amide group having from 2 to 20 carbon atoms, R2, R3, and R4 are each independently hydrogen or an acyl residue having from 1 to 6 carbon atoms, R5 is hydrogen, CH3, or CH2OH, and R6 is an organo group such as a hydrocarbon having from 1 to 10 carbon atoms are disclosed. Other seco-pseudopterosins and compds. related to pseudopterosins are disclosed. Examples are provided demonstrating the antiinflammatory, antiproliferative and analgesic activity of several compds. (pseudopterosin M, seco-pseudopterosin E, elisabethdione, etc.) isolated from *P. elisabethae*.

MSTR 2

L19 ANSWER 5 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

133:74170 MARPAT

TITLE:

Preparation of trienoic retinoid compounds with retinoic acid receptor and retinoid X receptor activity

INVENTOR(S):

Boehm, Marcus F.; Zhang, Lin; Nadzan, Alex M.

PATENT ASSIGNEE(S):

Ligand Pharmaceuticals Incorporated, USA

SOURCE:

U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 366,613, abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6083977	A	20000704	US 1995-481877	19950607
CA 2208981	AA	19960711	CA 1995-2208981	19951221
WO 9620913	A1	19960711	WO 1995-US16695	19951221
V: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LX, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9646430	A1	19960724	AU 1996-46430	19951221
AU 712187	B2	19991028		
EP 800503	A1	19971015	EP 1995-944360	19951221
EP 800503	B1	20000510		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE				
JP 10511948	T2	19981117	JP 1995-521088	19951221
CN 1220656	A	19990623	CN 1995-197736	19951221
CN 1121374	B	20030917		
AT 192731	F	20000515	AT 1995-944360	19951221
ES 2148593	T3	20001016	ES 1995-944360	19951221
NO 9703017	A	19970828	NO 1997-3017	19970627
US 1994-366613 19941230				
US 1995-480127 19950607				
US 1995-481877 19950607				
WO 1995-US16695 19951221				

PRIORITY APPLN. INFO.:

US 1994-366613 19941230

US 1995-480127 19950607

US 1995-481877 19950607

WO 1995-US16695 19951221

AB

Novel trienoic retinoid compds., e.g. of formula I (R1, R2, R4 = H, aryl, heteroaryl, CF3, alkyl, fluoroalkyl, perfluoroalkyl; R3 = H, CF3, alkyl, alkyl, fluoroalkyl, (substituted) OH; R5-R10 = H, alkyl, CF3; R11 = alkyl; X = (substituted) CO2H, (substituted) CONH2; Y = C, O, N, S), having activity for retinoic acid receptors and retinoid X receptors are prepd. Thus, II was prepd. from 3,5-di-tert-butylbenzoic acid and tri-Et 3-methyl-4-phosphonocrotonate in several steps. The IC50 of II was 253 nM against mitochondrial function of RPMI 8226 cell line. Pharmaceutical compns. contg. the title compds. and methods for their use are described.

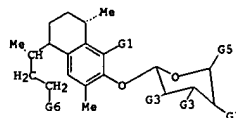
MSTR 2

G6-CH2-G4

G4 = 54

L19 ANSWER 4 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

(Continued)



G1 = OH

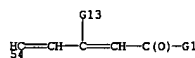
G6 = hydrocarbonyl&lt;(1-10)&gt;

MPL: claim 11

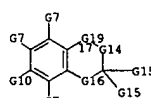
NTE: or pharmaceutically acceptable salts, prodrugs, or active metabolites

L19 ANSWER 5 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

(Continued)



G6 = 17



G7 = CF3

G10 = OH

G13 = Ak&lt;(1-4)&gt;

G14 = (0-2) 90



G15 = Ak&lt;(1-6)&gt;

G16 = 95



G19 = 123



MPL: claim 1

NTE: substitution is restricted

REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 131:58753 MARPAT  
 TITLE: 2,4,6-Trisubstituted pyridines with estrogenic activity and methods for the solid-phase synthesis thereof  
 INVENTOR(S): Chiu, Chingfan; Tang, Zhilian; Ellingboe, John Watson  
 PATENT ASSIGNEE(S): American Home Products Corporation, USA  
 SOURCE: PCT Int. Appl., 53 pp.  
 CODEN: PIXX02  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9932447	A2	19990701	WO 1998-US26363	19981210
WO 9932447	A3	19991014		

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9933528	A1	19990712	AU 1999-33528	19981210
US 6384060	B1	20020507	US 2000-703297	20001101
US 6384057	B1	20020507	US 2000-703386	20001101
US 6384058	B1	20020507	US 2000-703519	20001101
US 6503917	B1	20030107	US 2000-703508	20001101

PRIORITY APPLN. INFO.:

US 1997-109802P	19971211
US 1997-989057	19971211
US 1998-209663	19981210
WO 1998-US26363	19981210

AB The invention relates to (hydroxyaryl)pyridines I, II, and III [n = 1, 2; R1 = alkyl, cycloalkyl, Ph, R4C6H4 (R4 = H, F, Cl, Br, alkyl, cycloalkyl, alkoxy, methylenedioxy); R2 = furanyl, pyridyl, thienyl, naphthalenyl, Ph, R4C6H4; R3 = H, F, Cl, Br, NO2, alkyl, cycloalkyl, alkoxy], with estrogenic activity, to processes for their prep., to a combinatorial library and solid phase methods for prep. libraries of the compds., to utilizing libraries of the compds. for drug discovery, and to methods of treatment and pharmaceutical compns. thereof. Thus, condensation of Wang resin bound 2-HOC6H4COMe with 3,4-F3C6H3CHO gave resin-bound 2-HOC6H4COCH:CHC6H3F2-3,4 which condensed with 4-ClC6H4C(CH3)OSiMe3 to give resin-bound pentanedione IV. Cyclocondensation of IV with NH4OH and subsequent resin cleavage gave the trisubstituted pyridine V which at 1.µM possessed 14% estrogenic activity in an estrogen receptor assay.

MSTR 1

G1—G19

G1 = 29

L19 ANSWER 7 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 131:5112 MARPAT  
 TITLE: Preparation of N-[2-(1-naphthyl)ethyl]acetamides and analogs as melatonin receptor ligands  
 INVENTOR(S): Lefoulon, Francois; Demuynck, Luc; Lesieur, Daniel; Depreux, Patrick; Bennejean, Caroline; Renard, Pierre; Delagrang, Philippe  
 PATENT ASSIGNEE(S): Adir et Compagnie, Fr.  
 SOURCE: Eur. Pat. Appl., 44 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 919541	A1	19990602	EP 1998-402963	19981127

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

FR 2771739	A1	19990604	FR 1997-14975	19971128
FR 2771739	B1	20010420		

US 6143789	A	20001107	US 1998-199531	19981125
NO 9805516	A	19990531	NO 1998-5516	19981126

AU 9894213	A1	19990617	AU 1998-94213	19981127
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AU 757436	B2	20030220		
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CN 1221734	A	19990707	CN 1998-122715	19981127
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BR 9805031	A	20000328	BR 1998-5031	19981127
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NZ 333046	A	20000428	NZ 1998-333046	19981127
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JP 11263761	A2	19990928	JP 1998-338669	19981130
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ZA 9810872	A	19990601	ZA 1998-10872	19990601
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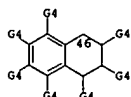
PRIORITY APPLN. INFO.:

AB R2Z1R1 [I: R = halo, alkyl, alkanoyloxy, aryl, etc.; R1 = NR2COR21, NR2CONHR21, CONR2R21, etc.; R2 = H or alkyl; R21 = alk(en)yl, aryl, C6H4Ph, etc.; Z = (un)substituted 2-8,1-naphthylene, -1,2-, -2,3- (sic), or -1,4-dihydronaphthylene; Z1 = (un)substituted alkylene] were prep. Thus, N-[2-(7-methoxy-1-naphthyl)ethyl]acetamide was converted in 4 steps to N-[2-(7-methoxy-3-phenyl-1-naphthyl)ethyl]acetamide. Data for biol. activity of I were given.

MSTR 5

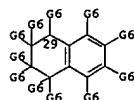
G1—G2—G7

G1 = 46

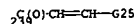


G2 = alkylene<(1-6)> (SO (1-) G3)  
 G4 = OH / 91

L19 ANSWER 6 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G5 = alkyl<(1-7)>  
 G19 = 239



G22 = OH  
 G25 = alkyl<(1-7)>  
 DER: and all crystalline forms and pharmaceutically acceptable salts  
 MPL: claim 1  
 NTE: substitution is restricted  
 NTE: also incorporates claim 19  
 STE: and enantiomers, racemic mixtures and diastereomeric mixtures

L19 ANSWER 7 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G6 = alkenyl<(2-6)> (SO)  
 MPL: claim 24

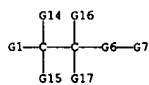
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 130:325148 MARPAT  
 TITLE: Preparation of heterocyclic compounds for the treatment of frequent urination or urinary incontinence  
 INVENTOR(S): Koga, Ichiro; Okada, Atsushi; Narita, Kazuhisa  
 PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 51 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

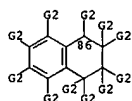
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9921839	A1	19990506	WO 1998-JP4807	19981023
W: AU, CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 407153	B	20001001	TW 1998-87117279	19981020
AU 9896469	A1	19990517	AU 1998-96469	19981023
PRIORITY APPLN. INFO.:				
JP 1997-309504 19971027				
WO 1998-JP4807 19981023				

AB The title compds. ArX(CH<sub>2</sub>)<sub>m</sub>B [Ar represents optionally substituted indanyl, naphthyl or tetrahydronaphthyl; X represents C(OH)R<sub>1</sub>CR<sub>2</sub>R<sub>3</sub> or CR<sub>1</sub>CR<sub>3</sub> (wherein R<sub>1</sub> represents hydrogen, lower alkyl, cycloalkyl or optionally substituted phenyl; and R<sub>2</sub> and R<sub>3</sub> are the same or different and each represents hydrogen or lower alkyl); m is an integer of 1 or 2; and B represents an optionally substituted heterocycle] are prepd. In a test for bladder contraction inhibition, the effect of trans-1-(4-methoxy-5,6,7,8-tetrahydro-1-naphthyl)-2-methyl-3-(2-methyl-1H-imidazol-1-yl)-1-propene hydrochloride was twice that of flavoxate hydrochloride in rats.

## MSTR 1



G1 = 86



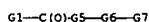
G2 = alkyl<(1-3)> (SO (1-) X) / OH / CH<sub>2</sub>Ph  
 G6 = (1-2) CH<sub>2</sub>

L19 ANSWER 9 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 130:139339 MARPAT  
 TITLE: Preparation of heterocyclic moiety-containing aromatic ketone derivatives for treatment of frequent urination or urinary incontinence  
 INVENTOR(S): Koga, Ichiro; Narita, Kazuhisa; Okada, Atsushi; Nakamura, Iwao  
 PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 61 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

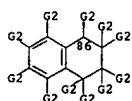
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9903835	A1	19990128	WO 1998-JP3179	19980715
W: AU, CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9882425	A1	19990210	AU 1998-82425	19980715
PRIORITY APPLN. INFO.:				
JP 1997-208378 19970718				
JP 1998-90699 19980320				
JP 1998-99915 19980330				
WO 1998-JP3179 19980715				

AB The title compds. ArCO(R<sub>1</sub>)(R<sub>2</sub>)(CH<sub>2</sub>)<sub>m</sub>BO (I) [Ar represents optionally substituted indanyl or tetrahydronaphthyl (excluding 5,6,7,8-tetrahydro-2-naphthyl); R<sub>1</sub> and R<sub>2</sub> are the same or different and each represents hydrogen or lower alkyl; m is 1 or 2; and BO represents an optionally substituted imidazolyl, imidazoliny, imidazolidiny, or triazolyl group] are prepd. I are calcium antagonists. In a test for bladder contraction inhibition, the effect of 1-(4-methoxy-5,6,7,8-tetrahydro-1-naphthyl)-2-methyl-3-(2-methyl-1H-imidazol-1-yl)-1-propanone hydrochloride was twice that of flavoxate hydrochloride in rats.

## MSTR 1



G1 = 86



G2 = alkyl<(1-3)> (SO (1-) X) / OH / CF<sub>3</sub> / hydrocarbyl<(1-10)>  
 DER: or pharmacologically acceptable salts  
 MPL: claim 1  
 NTE: also incorporates claim 11  
 NTE: substitution is restricted

REFERENCE COUNT: 23. THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS

L19 ANSWER 8 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)  
 G16 = alkyl<(1-6)>  
 DER: or pharmacologically acceptable salts  
 MPL: claim 1

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 127:262706 MARPAT  
 TITLE: Preparation of 2-amino-4-cycloalkylamino-1,3,5-triazines as herbicides and plant growth regulators  
 INVENTOR(S): Lorenz, Klaus; Minn, Klemens; Willms, Lothar; Bauer, Klaus; Bieringer, Hermann; Rosinger, Christopher  
 PATENT ASSIGNEE(S): Hoechst Schering Agrevo G.m.b.H., Germany  
 SOURCE: PCT Int. Appl., 92 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

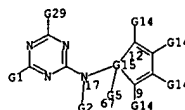
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731904	A1	19970904	WO 1997-EP702	19970214
V: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, YU				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19607450	A1	19970904	DE 1996-19607450	19960228
CA 2248338	AA	19970904	CA 1997-2248338	19970214
AU 9717693	A1	19970916	AU 1997-17693	19970214
AU 714187	B2	19991223		
EP 885201	A1	19981223	EP 1997-903284	19970214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI, RO				
CN 1212687	A	19990331	CN 1997-192683	19970214
CN 1083439	B	20020424		
BR 9707781	A	19990727	BR 1997-7781	19970214
JP 2000505462	T2	20000509	JP 1997-530544	19970214
US 6069114	A	20000530	US 1997-805576	19970225
ZA 9701642	A	19971125	ZA 1997-1642	19970226
DE 1996-19607450 19960228				
WO 1997-EP702 19970214				

PRIORITY APPLN. INFO.:

AB Title compds. [I; R1, R2 = H, (di) (alkyl) amino, hydrocarbyl, heterocyclyl, etc.; NR1R2 = heterocyclyl; R3, R5 = H, halo, cyano, hydrocarbyl(oxy), etc.; R4 = H, (di) (alkyl) amino, hydrocarbyl(oxy), etc.; R6 = H or 1-4 of halo, cyano, hydrocarbyl(oxy), etc.; R4 = H, (di) (alkyl) amino, hydrocarbyl(oxy), etc.; 2 = 1-4 of CH2, O, CO, (alkyl) imino, etc.; 21, 22 = bond, CH2, O, CO, (alkyl) imino, etc.] were prepd. as herbicides and plant growth regulators (no data). Thus, 1-amino-5,7-dimethyl-1,2,3,4-tetrahydronaphthalene hydrochloride was condensed with H2NC(=NH)NHCN.HCl and the product cyclocondensed with 2-FC6H4CO2Me to give title compd. II.

MSTR 1

L19 ANSWER 10 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G5 = Ak (SO)  
 G10 = O  
 G14 = CN  
 G15 = 105-17 107-12 105-67 106-9



G18 = 174

HC-G25  
T74

G25 = Me  
 DER: or salts  
 MPL: claim 1  
 NTE: substitution is restricted

L19 ANSWER 11 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

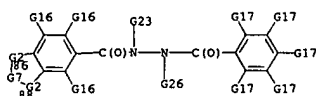
ACCESSION NUMBER: 127:19520 MARPAT  
 TITLE: Control of insects in fabrics by hydrazine derivatives  
 INVENTOR(S): Watabe, Tetsuo; Yamamoto, Yumiko  
 PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan; Sankyo Co., Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09100201	A2	19970415	JP 1995-256328	19951003
JP 1995-256328 19951003				

PRIORITY APPLN. INFO.:

AB Fabrics are protected from insects by hydrazine derivs. I (R1-4 = H, halo, Cl-4 alkyl, etc.; R5-7 = halo, nitro, cyano, Cl-4 alkyl, etc.; R8-10 = H, halo, Cl-4 alkyl, Cl-4 haloalkyl; R11 = H, cyano, etc.; R12 = C3-10 branched alkyl; p, m, n = 0,1), or other pesticides, insect repellents, microbicides, and dyes.

MSTR 1A



G2 = 11



G3 = alkyl<(1-4)>  
 G4 = acyl  
 G7 = 47-88 50-86



G16 = OH  
 MPL: claim 1  
 NTE: alkyl in G26 is branched  
 NTE: additional ring formation also claimed

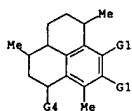
L19 ANSWER 11 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

L19 ANSWER 12 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 126:135635 MARPAT  
 TITLE: Use of pseudopterosins for promoting wound healing  
 INVENTOR(S): Haimes, Howard B.; Jimenez, Fabio A.  
 PATENT ASSIGNEE(S): Osteoarthritis Sciences, Inc., USA; Haimes, Howard B.; Jimenez, Fabio A.  
 SOURCE: PCT Int. Appl., 60 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640160	A1	19961219	WO 1996-US9039	19960606
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LX, LR, LS, LT, LU, LV, MD, MG, MK, MN, MV, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CH, GA				
US 5597808	A	19970128	US 1995-486359	19950607
CA 2223462	AA	19961219	CA 1996-2223462	19960606
AU 9661532	A1	19961230	AU 1996-61532	19960606
AU 707134	B2	19990701		
EP 831851	A1	19980401	EP 1996-919108	19960606
EP 831851	B1	20021120		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11506781	T2	19990615	JP 1996-501453	19960606
AT 227995	E	20021215	AT 1996-919108	19960606
US 6022862	A	20000208	US 1997-973126	19971203
PRIORITY APPLN. INFO.:			US 1995-486359	19950607
			WO 1996-US9039	19960606

AB Methods of promoting wound healing and the growth and proliferation of keratinocytes, fibroblasts and endothelial cells comprise contacting a wound with an effective wound healing amt. of a compn. comprising a pseudopterosin or pseudopterosin deriv. Thus, a pseudopterosin ointment contained pseudopterosin A Me ether 0.5, white petrolatum 84.0, white wax 10.0, cholesterol 3.0, and diisopropyl adipate 2.5. Several pseudopterosin alkyl ethers were prep'd. starting from pseudopterosin A. The effectiveness of pseudopterosin A Me ether in skin wound healing was demonstrated in guinea pigs.

MSTR 1



L19 ANSWER 13 OF 21 MARPAT COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 126:328301 MARPAT  
 TITLE: Preparation of N-phenalenylamides and analogs as melatonergic receptor ligands  
 INVENTOR(S): Langlois, Michel; Mathe-Allainmat, Monique; Delagrangue, Philippe; Renard, Pierre; Guardiola, Beatrice  
 PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.  
 SOURCE: Eur. Pat. Appl., 66 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 737670	A1	19961016	EP 1996-400777	19960411
EP 737670	B1	19990721		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
FR 2732964	A1	19961018	FR 1995-4503	19950414
FR 2732964	B1	19970516		
AT 182325	E	19990815	AT 1996-400777	19960411
ES 2136947	T3	19991201	ES 1996-400777	19960411
CA 2174034	AA	19961015	CA 1996-2174034	19960412
CA 2174034	C	20010102		
NO 9601456	A	19961015	NO 1996-1456	19960412
ZA 9602938	A	19961017	ZA 1996-2938	19960412
AU 9650628	A1	19961024	AU 1996-50628	19960412
AU 704261	B2	19990415		
JP 08291121	A2	19961105	JP 1996-91127	19960412
CN 1139666	A	19970108	CN 1996-105003	19960412
CN 1064349	B	20010411		
US 5712312	A	19980127	US 1996-631196	19960412
US 5849781	A	19981215	US 1997-942177	19971001
PRIORITY APPLN. INFO.:			FR 1995-4503	19950414
			US 1996-631196	19960412

AB Title compds. [e.g., I; R1-R4 = H, halo, alkyl, alkoxy, etc.; R5 = H, alkyl, aryl, etc.; R6 = alkanoyl, (alkyl)amino, etc.; R7,R8 = H, alkyl, alkoxy; Z = O, S, CH:CH, CH2CH2, etc.; dashed line = optional bond; n = 1-3] as melatonergic receptor ligands (no data). Thus, 1-chloromethylnaphthalene was alkylated by AcNHCH(CO2Et)2 and the decarboxylated product cyclized to give, after redn., title compd. II.

MSTR 1

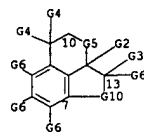
G1—G12—G16

G1 = 10

L19 ANSWER 12 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G1 = OH  
 G4 = Ak<(1-10)> (50 G9)  
 MPL: claim 1

L19 ANSWER 13 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G4 = alkyl<(1-6)>  
 G5 = (1-3) CH2  
 G6 = OH / alkyl<(1-6)> (50 (1-) X)  
 G10 = 95-7 96-13



DER: and pharmaceutically acceptable base addition salts  
 MPL: claim 1  
 NTE: substitution is restricted  
 STE: and enantiomers and diastereoisomers



L19 ANSWER 14 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 125:196058 MARPAT  
 TITLE: Preparation of new trienoic retinoid compounds and their activity toward retinoid receptors  
 INVENTOR(S): Boehm, Marcus F.; Zhang, Lin; Bennani, Youssef L.; Nadzan, Alex M.  
 PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA  
 SOURCE: PCT Int. Appl., 77 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9620913	A1	19960711	WO 1995-US16695	19951221
W:	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TH, TT			
RW:	KE, US, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
US 5721103	A	19980224	US 1995-480127	19950607
US 6083977	A	20000704	US 1995-481877	19950607
AU 9646430	A1	19960724	AU 1996-46430	19951221
AU 712187	B2	19991028		
EP 800503	A1	19971015	EP 1995-944360	19951221
EP 800503	B1	20000510		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE			
BR 9510414	A	19980519	BR 1995-10414	19951221
JP 10511948	T2	19981117	JP 1995-521088	19951221
AT 192731	E	20000515	AT 1995-944360	19951221
NO 9703017	A	19970828	NO 1997-3017	19970627

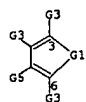
PRIORITY APPLN. INFO.:

AB The title compds., e.g., I (R1, R2, R4 = H, aryl, heteroaryl, (fluorinated) alkyl, labeled alkyl; R3, R5 = H, (fluorinated) alkyl, OH, alkoxy; R6 = (labeled) alkyl; R7 = alkyl; X = (substituted) CO2H, (substituted) CONH2), having activity for retinoic acid receptors and retinoid X receptors are prepd. Thus, II was prepd. in 5 steps from 3,5-di-tert-butylbenzoic acid. II showed a potency of <1 nM on retinoic acid receptor- $\gamma$ . Also provided are pharmaceutical compns. incorporating such compds. and methods for their use.

MSTR 3A

L19 ANSWER 14 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

L19 ANSWER 14 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G1 = 73-3 74-6



G2 = 116



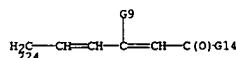
G3 = CF3  
 G5 = OH  
 G9 = Ak<(1-4)>  
 G19 = alkyl<(1-6)>  
 G20 = (1-3) 123



G26 = 158



G32 = 224



MPL: claim 1  
 NTE: substitution is restricted

L19 ANSWER 15 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

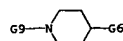
ACCESSION NUMBER: 122:205210 MARPAT  
 TITLE: Sigma receptor ligands, their preparation, and their therapeutic use  
 INVENTOR(S): Glennon, Richard A.; Fischer, James B.  
 PATENT ASSIGNEE(S): Cambridge Neuroscience, Inc., USA; Virginia Commonwealth University  
 SOURCE: PCT Int. Appl., 72 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9500131	A1	19950105	WO 1994-US7121	19940623
W:	AU, CA, CN, JP, KR, US			
RW:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			
CA 2166100	AA	19950105	CA 1994-2166100	19940623
AU 9471776	A1	19950117	AU 1994-71776	19940623
ZA 9404513	A	19960116	ZA 1994-4513	19940623
EP 714292	A1	19960605	EP 1994-920804	19940623
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			
US 6087346	A	20000711	US 1996-564362	19960221
			US 1993-82406	19930623
			WO 1994-US7121	19940623

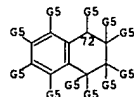
PRIORITY APPLN. INFO.:

AB Methods are disclosed for the treatment of central nervous system disorders, neurol. disorders, gastrointestinal disorders, drug abuse, angina, migraine, hypertension, and depression by administering a pharmaceutical compn. comprising an effective amt. of certain sigma receptor ligands (Markush included) to a patient in need of such treatment. Also disclosed are sigma receptor ligands having high binding to the sigma receptor, and pharmaceutical compns. thereof. Prepn. of selected compds. of the invention is described, and results of sigma-1 and sigma-2 binding assays are included.

MSTR 1



G2 = Ak<BD (0-) D (0) T> (SO OH)  
 G3 = 72



G5 = alkyl<(1-6)> / OH / CF3  
 DER: and pharmaceutically acceptable salts  
 MPL: claim 1

L19 ANSWER 15 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

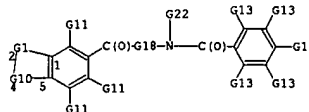
L19 ANSWER 16 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 122:125988 MARPAT  
 TITLE: Synergistic insecticides containing hydrazine and carbamate derivatives  
 INVENTOR(S): Watabe, Tetsuo; Kodama, Seichiro; Masui, Akio; Yokoi, Shinji; Ichinose, Reiji  
 PATENT ASSIGNEE(S): Nippon Kayaku Kk, Japan; Sankyo Co  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
 CODEN: JKOXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06256108	A2	19940913	JP 1993-43815	19930304
PRIORITY APPLN. INFO.:				
			JP 1993-43815	19930304

AB A synergistic compn. contains I [N-(5-methyl-1,4-benzodioxan-6-carbo)-N'-t-butyl-N''-(3,5-dimethylbenzoyl)hydrazine], or its derivs. (Markush structure given), in combination with a carbamate deriv. like pyrimicarb to control insects (e.g., *Pletella maculipennis*).

MSTR 1B



G1 = 10-4 11-1



G2 = 14



G5 = alkyl<(1-4)> / acyl  
 G10 = 97-2 98-5

L19 ANSWER 16 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G11 = OH  
 MPL: claim 1  
 NTE: alkyl in G22 is branched

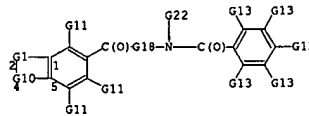
L19 ANSWER 17 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 122:74622 MARPAT  
 TITLE: Synergistic insecticides containing hydrazine derivatives  
 INVENTOR(S): Watabe, Tetsuo; Kodama, Seichiro; Masui, Akio; Yokoi, Shinji; Ichinose, Reiji  
 PATENT ASSIGNEE(S): Nippon Kayaku Kk, Japan; Sankyo Co  
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
 CODEN: JKOXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06298609	A2	19941025	JP 1993-92997	19930420
PRIORITY APPLN. INFO.:				
			JP 1993-92997	19930420

AB A synergistic insecticide contains a hydrazine deriv. (Markush structure given) such as N-(5-methyl-1,4-benzodioxan-6-carbo)-N'-t-butyl-N''-(3,5-dimethylbenzoyl)hydrazine (I) and a compd. selected from the group comprising nitromethylene compds., nitroguanidine compds., imidazolidine compds., tetrahydropyrimidine compds. and amidine compds. Insecticidal activities of the mixts. against *Plutella xylostella* (cabbage moth) were demonstrated.

MSTR 1B



G1 = 10-4 11-1



G2 = 14



G5 = alkyl<(1-4)> / acyl  
 G10 = 97-2 98-5

L19 ANSWER 17 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



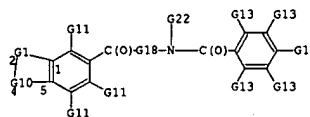
G11 = OH  
 MPL: claim 1  
 NTE: alkyl in G22 is branched

L19 ANSWER 18 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 122:25899 MARPAT  
 TITLE: Insecticides containing hydrazine and pyrethroid compounds  
 INVENTOR(S): Watabe, Tetsuo; Kodama, Seichiro; Masui, Akio; Yokoi, Shinji; Ichinose, Reiji  
 PATENT ASSIGNEE(S): Nippon Kayaku Kk, Japan; Sankyo Co  
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
 CODEN: JKOXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06263604	A2	19940920	JP 1993-53703	19930315
PRIORITY APPLN. INFO.:				
AB An insecticide contains a hydrazine deriv. [e.g., N-(5-methylcroman-6-carboxyl)-N'-t-butyl-N'-(3,5-dimethylbenzoyl)hydrazine (I)] (Markush structures given) and storeq. 1 pyrethroid compd. [e.g., etofenprox]. The mixt. is effective in controlling insects like beetles and Plutella xylostella. In the rice paddy, the mixt. is effective against both Chilo suppressalis and Nilaparvata lugens.				

MSTR 15



G1 = 10-4 11-1



G2 = 14



G5 = alkyl&lt;(1-4)&gt; / acyl

L19 ANSWER 18 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G11 = OH  
 MPL: claim 1  
 NTE: alkyl in G22 is branched

L19 ANSWER 19 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

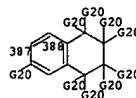
ACCESSION NUMBER: 119:116944 MARPAT  
 TITLE: Preparation of o-hydroxynitroso aromatic compound-metal complexes  
 INVENTOR(S): Nakamura, Masataka; Taniguchi, Takashi  
 PATENT ASSIGNEE(S): Toray Industries, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKOXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05032591	A2	19930209	JP 1991-194382	19910802
PRIORITY APPLN. INFO.:				
AB The title compds. [I-metal complex; R1 = HO, (un)substituted NH2, C1-20 alkoxy or acyloxy, C7-15 aralkoxy or aralkyl, C6-14 aryloxy, C2-20 alkenyl or alkynyl, C1-20 carbamoyl or alkoxy-sulfonyl, etc.], n = 0-3; X = (un)substituted NH2, C1-20 alkoxy, C6-14 aryloxy or arylthio, C7-15 aralkoxy or aralkylthio; ring .alpha. = absent or a C3-18 ring], useful as intermediates for functional dyes, are prepd. by reaction of I-metal complex (X = H) with HX (X = same as above). Thus, 20.4 g 1-nitroso-2-naphthol-Cu complex and 5.4 g NaOMe were refluxed in 400 ml anhyd. MeOH for 3 h to give 4-ethoxy-1-nitroso-2-naphthol-Cu complex which (I g) was refluxed with 1 g 1,3,3-trimethyl-2-methyleneindoline in 20 ml EtOH for 20 h to give a spiro[indoline-naphthoxazine] deriv. (II; R2 = OEt). Also prepd. were 1-nitroso-4-piperidino-2-naphthol-Cu complex and II (R2 = piperidino).				

MSTR 15



G1 = 388-3 387-1



G20 = alkyl<(1-20)> / alkenyl<(2-20)> / CN  
 MPL: claim 1

L19 ANSWER 20 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 119:52681 MARPAT  
 TITLE: Two-cycle lubricants and methods of using them  
 INVENTOR(S): Blythe, Glen H.  
 PATENT ASSIGNEE(S): Lubrizol Corp., USA  
 SOURCE: PCT Int. Appl., 69 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

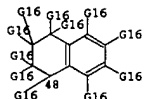
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9303120	A1	19930218	WO 1992-US6040	19920721
W: AU, BR, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
US 5264005	A	19931123	US 1991-744618	19910809
AU 9223741	A1	19930302	AU 1992-23741	19920721
AU 656018	B2	19950119		
EP 552334	A1	19930728	EP 1992-916253	19920721
EP 552334	B1	19980812		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
AT 169664	E	19980815	AT 1992-916253	19920721
ES 2123003	T3	19990101	ES 1992-916253	19920721
IL 102664	A1	19950526	IL 1992-102664	19920728
ZA 9205942	A	19930428	ZA 1992-5942	19920807
CN 1073200	A	19930616	CN 1992-110633	19920808
CN 1034020	B	19970212		

PRIORITY APPLN. INFO.:  
 US 1991-744618 19910809  
 WO 1992-US6040 19920721  
 AB A fuel-lubricant mixt. for two-cycle internal-combustion engines comprises a major amt. of a fuel and a minor amt. sufficient to increase compression or release stuck piston rings, of a lubricant compn. comprising (A) .gtoreq.1 dispersant, (B) .gtoreq.1 reaction product of a fatty acid and a polyamine, optionally treated with an alkylene oxide, (C) .gtoreq.1 varnish dissolver selected from (1) keto alcs., (2) C.ltoreq.24 carboxylic esters, and (3) alkoxy alcs., and (D) .ltoreq.15 wt.% of the compn. of .gtoreq.1 fluidizing oil. The compn. also improves general engine cleanliness of two-cycle engines.

MSTR 1A

G3—G1

G1 = 48



L19 ANSWER 21 OF 21 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 110:4187 MARPAT  
 TITLE: Composition and method for rapid differentiation of viable fungi from bacteria using polyene antibiotics  
 INVENTOR(S): Cichanowicz, Peggy Woodruff; Belly, Robert Troconis  
 PATENT ASSIGNEE(S): Eastman Kodak Co., USA  
 SOURCE: Eur. Pat. Appl., 22 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

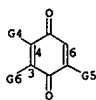
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 261931	A2	19880330	EP 1987-308380	19870922
EP 261931	A3	19891011		
R: CH, DE, FR, GB, LI				
CA 1290226	A1	19911008	CA 1986-523203	19861118
PRIORITY APPLN. INFO.: US 1986-910923 19860924				

AB Viable fungi are rapidly differentiated from viable bacteria by incubation with a compn. contg. a polyene antibiotic which affects membrane function in fungi and a compd. [e.g. a RIND compd. (reducible compd. which undergoes intramol. nucleophilic displacement) such as quinone I, where R1 = (R5)m(R6)QX; R2, R4 = H, (substituted) alkyl or aryl, electron-withdrawing group; R3 = R1, R2; or R3R4 complete a (substituted) strained fused carbocyclic ring; R5 = (substituted) C1-2 alkylene; R6 = (substituted) alkyl, cycloalkyl, aryl, or heterocycle; Q = C(O), C(S); X = shiftable detectable species which provides a detectable species when released; m = 0, 1] which is normally reducible by both fungi and bacteria. The antibiotic selectively inhibits the redn. of the reducible compd. by the fungi but does not affect the reducing capacity of the bacteria. A soln. contg. RIND compd. II, glucose, trimethyl-1,4-benzoquinone (electron transfer agent), buffer, and filipin (polyene antibiotic) at various dilns. was incubated with suspensions of various bacteria and fungi at 37.degree. for 30 min, and the difference in relative fluorescence before and after incubation was measured with excitation at 540 nm and emission at 620 nm. The percent inhibition of redn. of II at 0.52 mg filipin/mL was: Escherichia coli, 0; Staphylococcus aureus, 8.6; Candida albicans, 71.0; Aspergillus flavus, 42.5.

MSTR 1B

G2—G1

G1 = 6

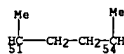


G5 = OMe  
 G7 = alkylene<(1-2)> (SO (1-) G11)  
 G4 + G6 = 51-4 54-3

L19 ANSWER 20 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G3 = Ak<(10-400)> (SO (1-) G15)  
 G16 = OH / Ak<(10-400)> (SO)  
 MPL: claim 2  
 NTE: substitution is restricted

L19 ANSWER 21 OF 21 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



MPL: claim 4

=> d his

(FILE 'HOME' ENTERED AT 12:28:21 ON 14 OCT 2003)

FILE 'REGISTRY' ENTERED AT 12:28:26 ON 14 OCT 2003

L1               STRUCTURE UPLOADED  
L2               7 S L1 FULL  
L3               STRUCTURE UPLOADED  
L4               11 S L3 FULL  
L5               STRUCTURE UPLOADED  
L6               34 S L5 FULL  
L7               STRUCTURE UPLOADED  
L8               0 S L7 FULL  
L9               52 S L2 OR L4 OR L6

FILE 'CAPLUS' ENTERED AT 12:33:01 ON 14 OCT 2003

L10              41 S L9  
L11              34 S L10 NOT PY>=2002  
L12              3 S L9/USES

FILE 'BEILSTEIN' ENTERED AT 12:53:20 ON 14 OCT 2003

L13              5 S L1 FULL  
L14              6 S L3 FULL  
L15              23 S L5 FULL

FILE 'MARPAT' ENTERED AT 12:55:16 ON 14 OCT 2003

L16              2 S L2 FULL  
L17              3 S L4 FULL  
L18              18 S L6 FULL  
L19              21 S L16 OR L17 OR L18